

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Dawn Garrett Examiner #: 76107 Date: 4/23/2003
 Art Unit: 1774 Phone Number 272-1523 Serial Number: 101634755
 Mail Box and Bldg/Room Location: Results Format Preferred (circle): PAPER DISK E-MAIL
Romeen 5C75

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Organic Electroluminescent Device Based on Pyrene Derivatives

Inventors (please provide full names): Xiao-Chang Li, Yoshimasa Okamura, Kazunori Ueno,
Masashi Tashiro, Hideki Tashiro, G.K. Prakash

Earliest Priority Filing Date: 8/6/2003

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search compound of claim 1
 (the compound must contain at least one
 deuterium atom)

(No EL-RELATED ART OUT THERE.)

STAFF USE ONLY

Searcher: ED

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: 4-23-04

Searcher Prep & Review Time: 10

Clerical Prep Time: _____

Online Time: 70

Type of Search

NA Sequence (#) _____ STN \$ 318.65

AA Sequence (#) _____ Dialog _____

Structure (#) (1) Questel/Orbit _____

Bibliographic (and) Dr. Link _____

Litigation _____ Lexis/Nexis _____

Fulltext _____ Sequence Systems _____

Patent Family _____ WWW/Internet _____

Other _____ Other (specify) _____

=> file reg

FILE 'REGISTRY' ENTERED AT 20:04:04 ON 23 APR 2004
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FILE 'LREGISTRY' ENTERED AT 19:55:24 ON 23 APR 2004
E PYRENE/CN

L1 1 S E3
L2 62 S 3593.5.31/RID
L3 1 S L2 AND D/ELS

FILE 'REGISTRY' ENTERED AT 19:55:59 ON 23 APR 2004
L4 114 S L3

FILE 'HCA' ENTERED AT 19:56:36 ON 23 APR 2004

L5 130 S L4
L6 82576 S (ELECTROLUM!N? OR ORGANOLUM!N? OR (ELECTRO OR ORGANO OR
L7 0 S L5 AND L6

FILE 'HCAPLUS' ENTERED AT 19:57:40 ON 23 APR 2004

L8 6799 S TASHIRO ?/AU
L9 5737 S PRAKASH ?/AU
L10 6 S L8 AND L9
SEL L10 1-6 RN

FILE 'REGISTRY' ENTERED AT 19:58:08 ON 23 APR 2004

L11 150 S E1-E150
L12 0 S L11 AND L4
L13 0 S L11 AND D/ELS
L14 0 S L11 AND L2

FILE 'HCAPLUS' ENTERED AT 19:59:03 ON 23 APR 2004

L15 0 S L10 AND L6

FILE 'REGISTRY' ENTERED AT 19:59:47 ON 23 APR 2004

L16 28 S L4 AND 1<NRS
L17 74096 S (T OR TERT OR TERTIAR?) (A) BUTYL?
L18 0 S L4 AND L17
E PYRENE-D10/CN
L19 1 S E3
L20 113 S L4 NOT L19

FILE 'HCA' ENTERED AT 20:01:50 ON 23 APR 2004

L21 39 S L20
 L22 11 S L16
 L23 11 S L22 AND L21
 L24 11 S L23 OR L22
 L25 28 S L21 NOT L24
 L26 91 S L5 NOT (L24 OR L25)

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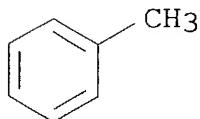
=> d 124 1-11 cbib abs hitstr hitrn

L24 ANSWER 1 OF 11 HCA COPYRIGHT 2004 ACS on STN
 140:121462 Pyrene-bridged bis(phenanthroline) ligands and their
 dinuclear ruthenium(II) complexes. Chouai, Latif; Wu, Feiyue; Jang,
 Youngchan; Thummel, Randolph P. (Department of Chemistry, University
 of Houston, Houston, TX, 77204-5003, USA). European Journal of
 Inorganic Chemistry (15), 2774-2782 (English) 2003. CODEN: EJICFO.
 ISSN: 1434-1948. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA.
 AB The Friedlaender condensation of 8-amino-7-quinolinicarbaldehyde
 with four isomeric diacetylpyrenes provides the corresponding 1,3-,
 1,6-, 1,8-, and 2,7-bis(2'-[1',10']phenanthrolinyl)pyrenes. These
 ligands, along with the tetrahydro analog to the 2,7-pyrene-bridged
 isomer, were treated with [Ru([D8]bpy)2Cl2], where [D8]bpy =
 [D8]2,2'-bipyridine, to afford the dinuclear RuII complexes, 1H NMR
 and x-ray crystallog. anal. of which indicate that the bridging
 pyrene is layered between a [D8]bpy auxiliary ligand coordinated to
 each metal atom. Although well situated for π - π interactions,
 little such effect is seen on the photophys. and electrochem.
 properties of these complexes.
 IT 646035-00-9P
 (prepn. and crystal structure of)
 RN 646035-00-9 HCA
 CN Ruthenium(4+), tetrakis(2,2'-bipyridine-3,3',4,4',5,5',6,6'-d8-
 κ N1, κ N1') [μ -[2,2'-(1,6-pyrenediyl)bis[1,10-
 phenanthroline- κ N1, κ N10]]]di-,
 tetrakis[hexafluorophosphate(1-)], compd. with acetonitrile,
 dichloromethane and methylbenzene (1:4:2:2) (9CI) (CA INDEX NAME)

CM 1

CRN 108-88-3

CMF C7 H8



CM 2

CRN 75-09-2
CMF C H2 Cl2Cl—CH₂—Cl

CM 3

CRN 75-05-8
CMF C2 H3 NH₃C—C≡N

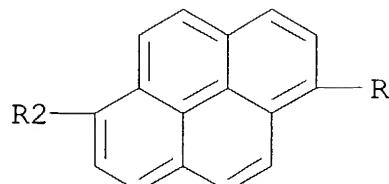
CM 4

CRN 646034-95-9
CMF C80 H22 D32 N12 Ru2 . 4 F6 P

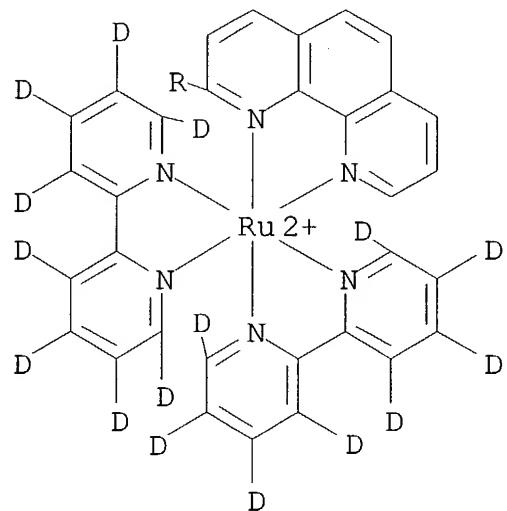
CM 5

CRN 646034-94-8
CMF C80 H22 D32 N12 Ru2
CCI CCS

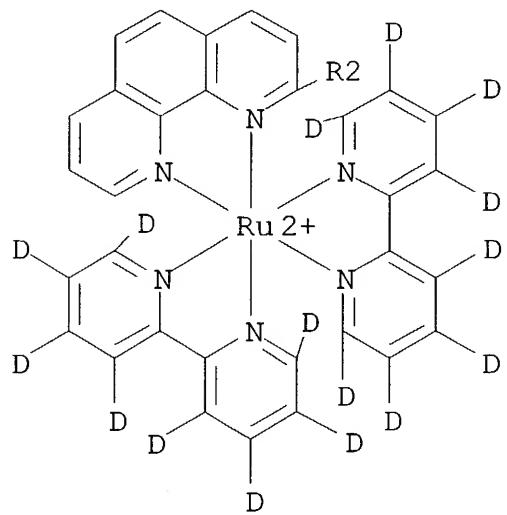
PAGE 1-A



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PAGE 3-A

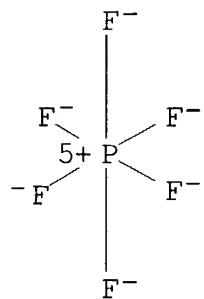


CM 6

CRN 16919-18-9

CMF F6 P

CCI CCS



IT 646034-93-7P 646034-97-1P 646034-99-3P
 (prepn. and cyclic voltammetry and luminescence spectra and
 electronic spectra)

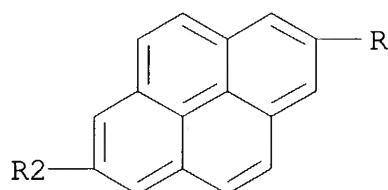
RN 646034-93-7 HCA

CN Ruthenium(4+), tetrakis(2,2'-bipyridine-3,3',4,4',5,5',6,6'-d8-
 κN1,κN1') [μ-[2,2'-(2,7-pyrenediyl)bis[1,10-
 phenanthroline-κN1,κN10]]]di-,
 tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

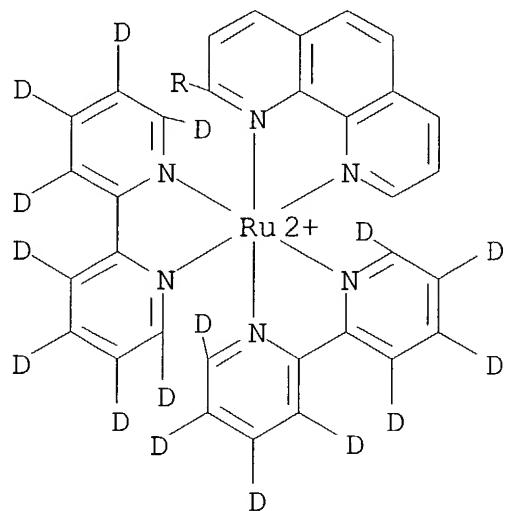
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CRN 646034-92-6
 CMF C80 H22 D32 N12 Ru2
 CCI CCS

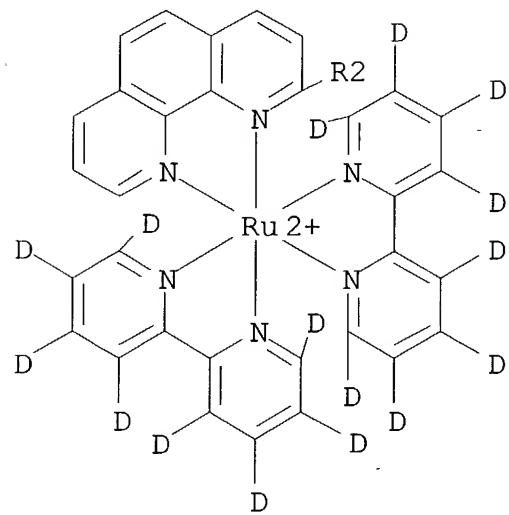
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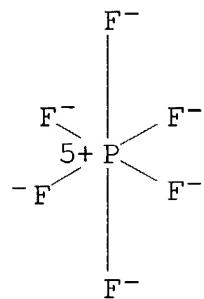


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



RN 646034-97-1 HCA

CN Ruthenium(4+), tetrakis(2,2'-bipyridine-3,3',4,4',5,5',6,6'-d8-
κN1,κN1') [μ-[2,2'-(1,8-pyrenediyl)bis[1,10-
phenanthroline-κN1,κN10]]]di-,
tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

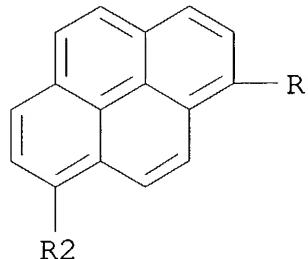
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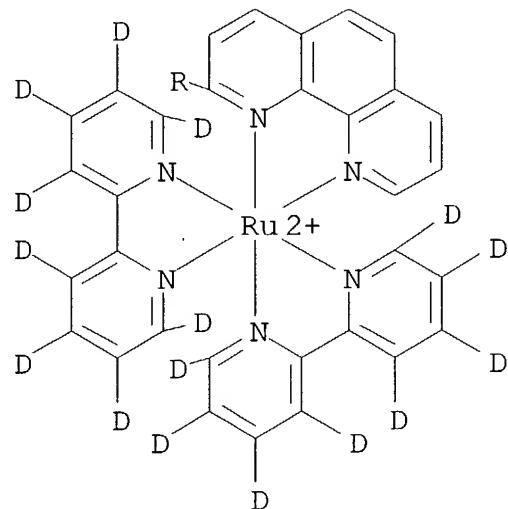
CMF C80 H22 D32 N12 Ru2

CCI CCS

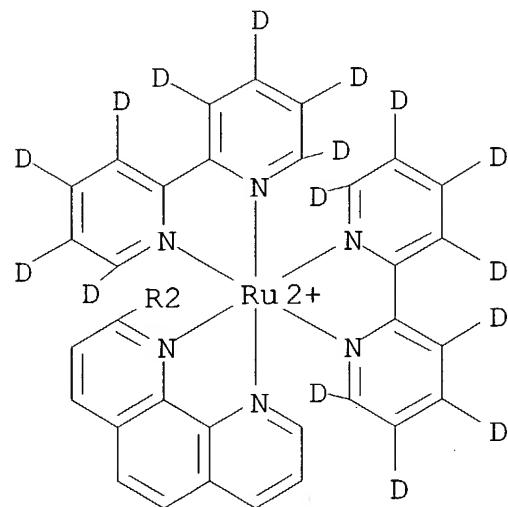
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PAGE 2-A



PAGE 3-A

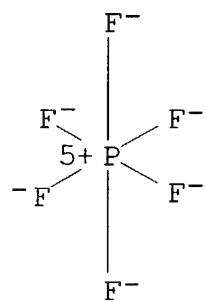


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



RN 646034-99-3 HCA

CN Ruthenium(4+), tetrakis(2,2'-bipyridine-3',4,4',5,5',6,6'-d8-
κN1,κN1') [μ-[2,2'-(1,3-pyrenediyl)bis[1,10-
phenanthroline-κN1,κN10]]]di-,
tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

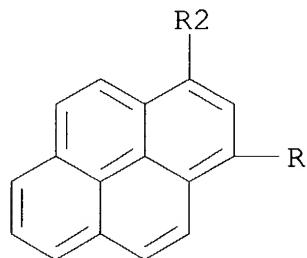
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CRN 646034-98-2

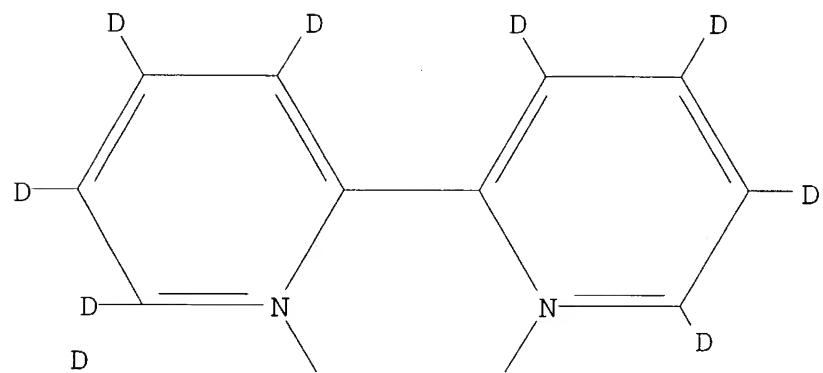
CMF C80 H22 D32 N12 Ru2

CCI CCS

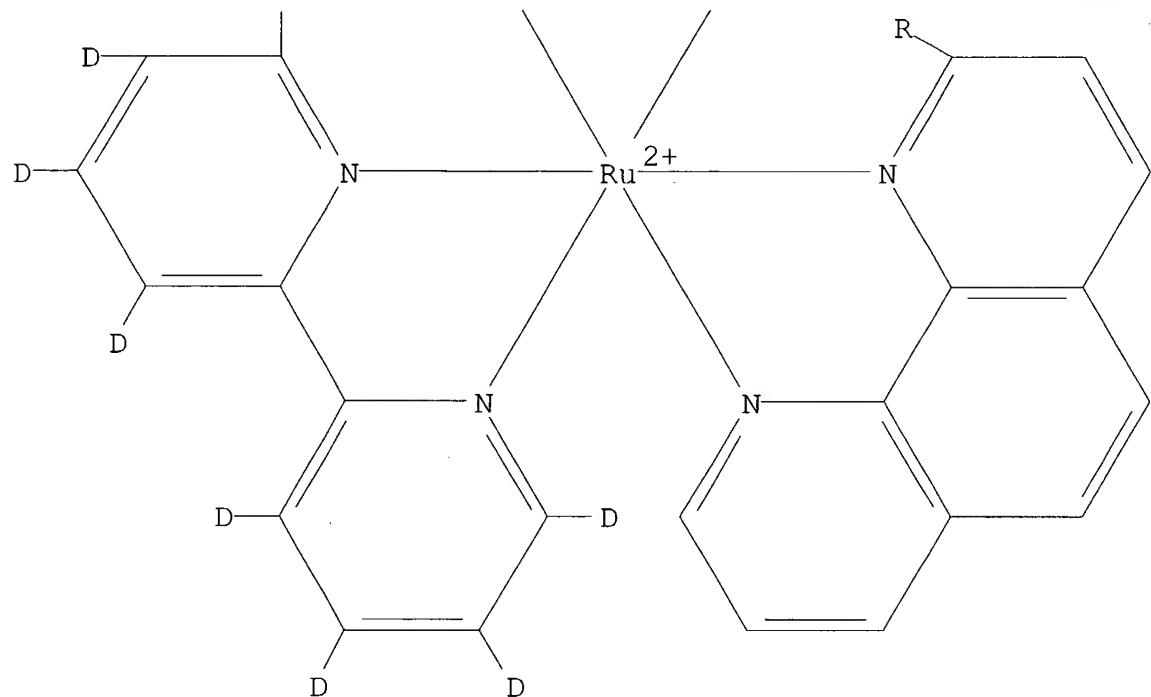
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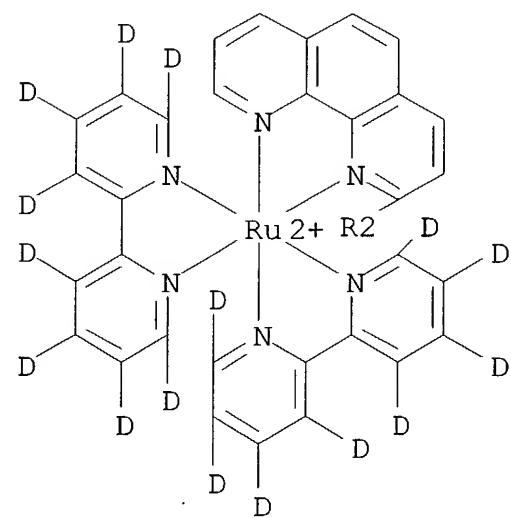
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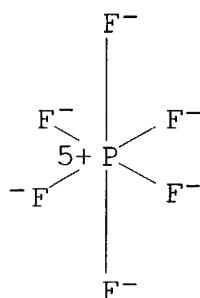


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



IT 646034-95-9P

(prepn. and cyclic voltammetry and luminescence spectra and electronic spectra and crystal structure)

RN 646034-95-9 HCA

CN Ruthenium(4+), tetrakis(2,2'-bipyridine-3',4,4',5,5',6,6'-d8-
 κ N1, κ N1') [μ -[2,2'-(1,6-pyrenediyl)bis[1,10-
 phenanthroline- κ N1, κ N10]]]di-,
 tetrakis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

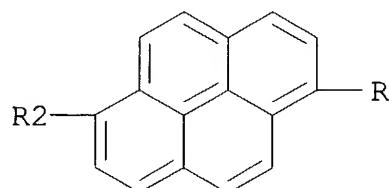
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CRN 646034-94-8

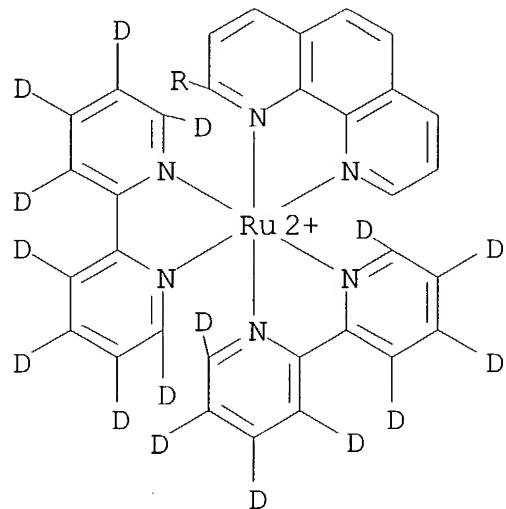
CMF C80 H22 D32 N12 Ru2

CCI CCS

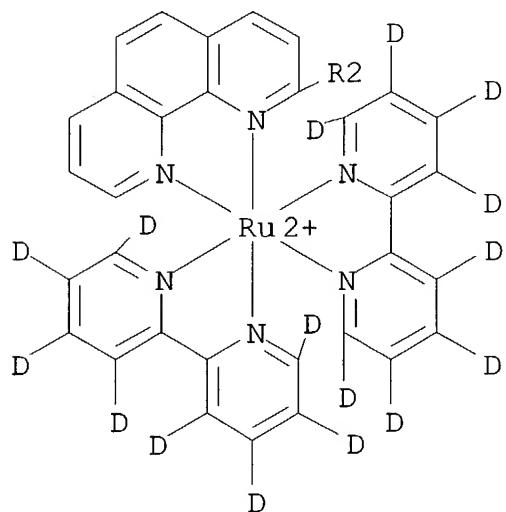
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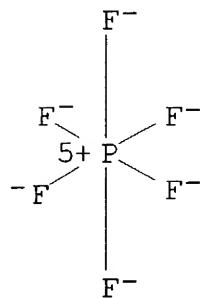


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



IT 646035-00-9P
 (prepn. and crystal structure of)

IT 646034-93-7P 646034-97-1P 646034-99-3P
 (prepn. and cyclic voltammetry and luminescence spectra and electronic spectra)

IT 646034-95-9P
 (prepn. and cyclic voltammetry and luminescence spectra and electronic spectra and crystal structure)

L24 ANSWER 2 OF 11 HCA COPYRIGHT 2004 ACS on STN

133:252140 A New Case of Chiral Recognition between Isotopomers.

Preparation and Study of (R) and (S) Perdeuterio

2,2,2-Trifluoro-1-(1-pyrenyl)ethanol. Munoz, Anna; Sanchez, Marta;

Junk, Thomas; Virgili, Albert (Unitat de Quimica Organica

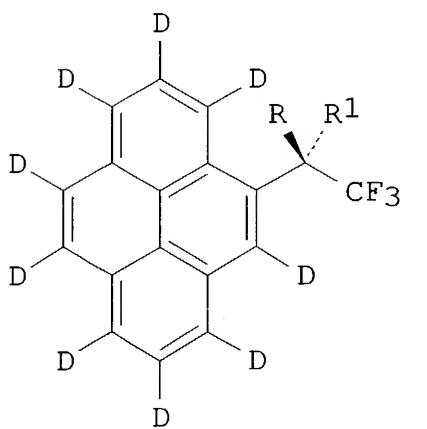
Departament de Quimica, Universitat Autonoma de Barcelona,

Barcelona, 08193, Spain). Journal of Organic Chemistry, 65(16),

5069-5071 (English) 2000. CODEN: JOCEAH. ISSN: 0022-3263.

Publisher: American Chemical Society.

GI



AB Perdeuteriopyrenyltrifluoroethanol I (R = H, HO; R1 = HO, H) is prep'd. and sep'd. into its enantiomers. (S)-(+)-I (R = HO; R1 = H) acts as a chiral shift reagent for its nondeuterated isotopomer; peaks for the (S)-enantiomer of the nondeuterated isotopomer are shifted to lower field than the corresponding protons in the (R)-enantiomer.

IT 295429-60-6 295429-66-2
(mol. mechanics calcns. of the complex of a chiral shift reagent with the enantiomers of its nondeuterated isotopomer)

RN 295429-60-6 HCA

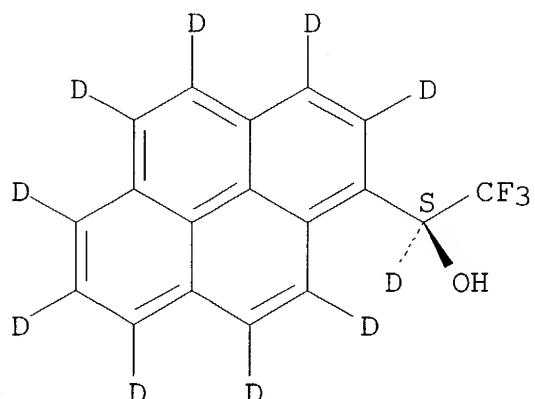
CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d9-methan- α -d-ol,
 α -(trifluoromethyl)-, (α S)-, compd. with
(α S)- α -(trifluoromethyl)-1-pyrenemethanol (1:1) (9CI)
(CA INDEX NAME)

CM 1

CRN 295429-50-4

CMF C18 H D10 F3 O

Absolute stereochemistry. Rotation (+).

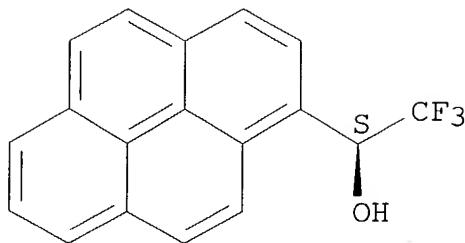


CM 2

CRN 187840-12-6

CMF C18 H11 F3 O

Absolute stereochemistry. Rotation (+).



RN 295429-66-2 HCA

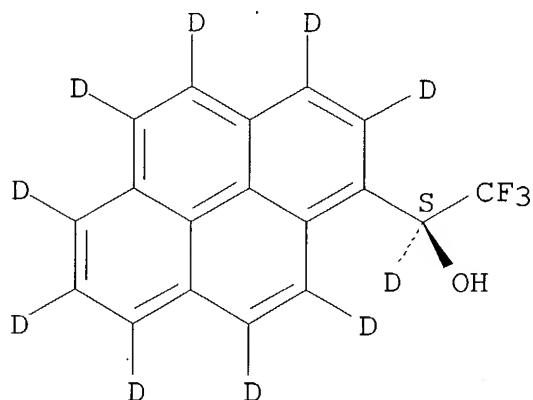
CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d9-methan- α -d-ol,
 α -(trifluoromethyl)-, (α S)-, compd. with
 $(\alpha$ R)- α -(trifluoromethyl)-1-pyrenemethanol (1:1) (9CI)
(CA INDEX NAME)

CM 1

CRN 295429-50-4

CMF C18 H D10 F3 O

Absolute stereochemistry. Rotation (+).

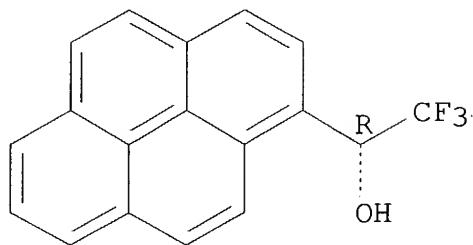


CM 2

CRN 73048-51-8

CMF C18 H11 F3 O

Absolute stereochemistry. Rotation (-).



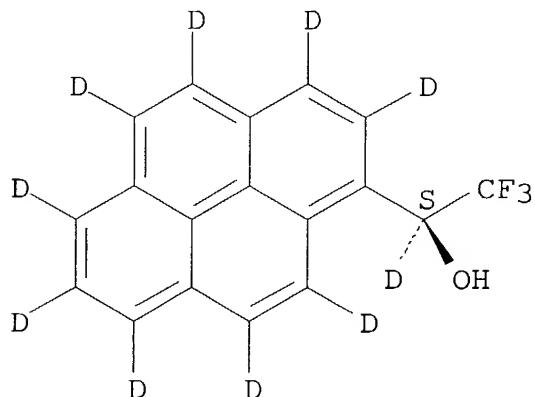
IT 295429-50-4P

(prepn. of nonracemic perdeuteriopyrenyltrifluoroethanol as a chiral shift reagent for its nondeuterated isotopomer)

RN 295429-50-4 HCA

CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d9-methan-alpha-d-ol,
alpha-(trifluoromethyl)-, (alphaS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

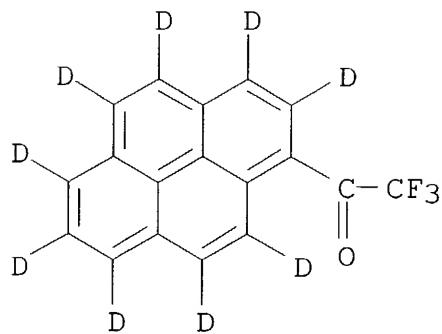


IT 295429-35-5P 295429-40-2P

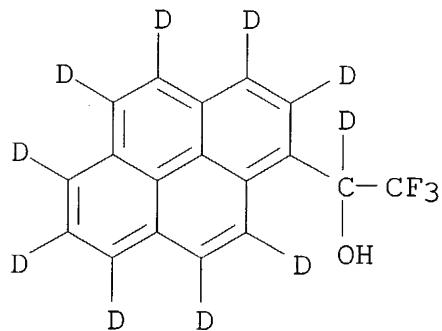
(prepn. of nonracemic perdeuteriopyrenyltrifluoroethanol as a chiral shift reagent for its nondeuterated isotopomer)

RN 295429-35-5 HCA

CN Ethanone, 2,2,2-trifluoro-1-(1-pyrenyl-2,3,4,5,6,7,8,9,10-d9)- (9CI)
(CA INDEX NAME)



RN 295429-40-2 HCA

CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d9-methan-alpha-d-ol,
alpha-(trifluoromethyl)- (9CI) (CA INDEX NAME)

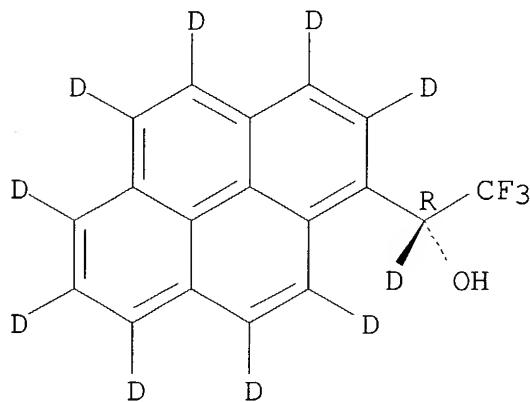
IT 295429-45-7P

(prepn. of nonracemic perdeuteriopyrenyltrifluoroethanol as a
chiral shift reagent for its nondeuterated isotopomer)

RN 295429-45-7 HCA

CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d9-methan-alpha-d-ol,
alpha-(trifluoromethyl)-, (alphaR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 295429-60-6 295429-66-2

(mol. mechanics calcns. of the complex of a chiral shift reagent with the enantiomers of its nondeuterated isotopomer)

IT 295429-50-4P

(prepn. of nonracemic perdeuteriopyrenyltrifluoroethanol as a chiral shift reagent for its nondeuterated isotopomer)

IT 295429-35-5P 295429-40-2P

(prepn. of nonracemic perdeuteriopyrenyltrifluoroethanol as a chiral shift reagent for its nondeuterated isotopomer)

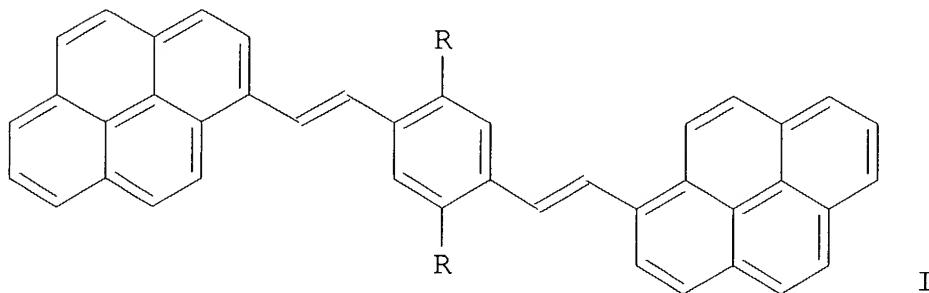
IT 295429-45-7P

(prepn. of nonracemic perdeuteriopyrenyltrifluoroethanol as a chiral shift reagent for its nondeuterated isotopomer)

L24 ANSWER 3 OF 11 HCA COPYRIGHT 2004 ACS on STN

128:61225 Electronic characteristics of large π -electron conjugated dumbbell-shaped donors and their radial cationic salts. Mizutani, Makoto (Central Res. Laboratories, Idemitsu Kosan Co., Ltd., Chiba, 299-02, Japan). Advances in Colloid and Interface Science, 71-72, 111-124 (English) 1997. CODEN: ACISB9. ISSN: 0001-8686.
Publisher: Elsevier.

GI



AB We investigated the new concept of donors in the synthesis of org. metals. We studied two dumbbell-shaped donors, trans,trans-1,4-bis[2-(1-pyrenyl)ethenyl]-2,5-dimethylbenzene (BPE-DMB), and -1,4-bis[2-(1-pyrenyl)ethenyl]benzene (BPE-B) (I; R = Me and H, resp.) and found that they have good solv. in spite of extended π -electron conjugation. These donors were easily formed into highly conductive salts; for example, dibromoiode (IBr₂) salts had conductivities as high as 100 S/cm at room temp. Above 220 K, the (BPE-DMB) (IBr₂) salt showed metallic conducting behavior. We used the electron resonance spectra and the reflectance spectra of these salts to examine metallic properties at this temp. Furthermore, IR spectra showed that the π -electron conjugation of BPE-DMB extended over the entire mol. in the salt. Therefore, it appeared that the (BPE-DMB) (IBr₂) salt was novel one which exhibited a metallic state in spite of the donor being in a monocation.

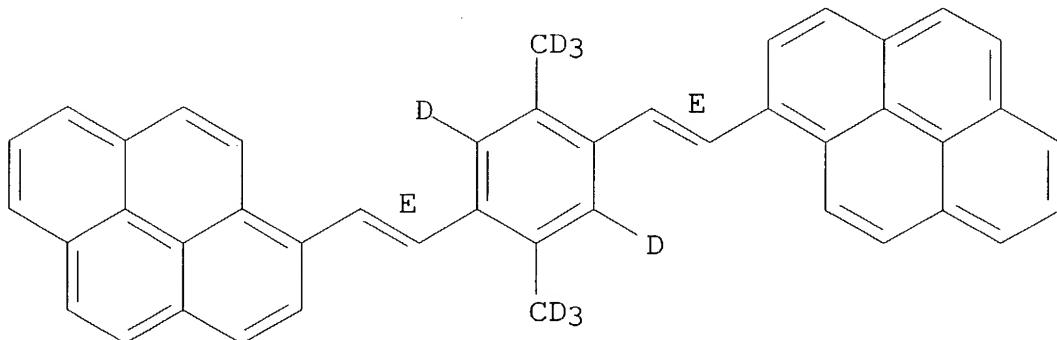
IT 200336-98-7P

(electronic characteristics of large π -electron conjugated dumbbell-shaped donors and their radial cationic salts)

RN 200336-98-7 HCA

CN Pyrene, 1,1'-[[3,6-di(methyl-d3)-1,4-phenylene-2,5-d2]di-2,1-ethenediyl]bis-, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 200336-98-7P

(electronic characteristics of large π -electron conjugated dumbbell-shaped donors and their radial cationic salts)

L24 ANSWER 4 OF 11 HCA COPYRIGHT 2004 ACS on STN

124:316421 Exceptionally persistent and oxygen-insensitive

2,7-di-tert-butylpyren-1-oxyl radical: synthesis, dimerization, EPR and ENDOR Spectra. Miura, Yozo; Yamano, Eiji; Miyazawa, Akira; Tashiro, Masashi (Dep. Applied Chemistry, Osaka City Univ., Osaka, 558, Japan). Journal of the Chemical Society, Perkin Transactions

2: Physical Organic Chemistry (3), 359-64 (English) 1996. CODEN: JCPKBH. ISSN: 0300-9580. OTHER SOURCES: CASREACT 124:316421. Publisher: Royal Society of Chemistry.

AB Oxidn. of 2,7-di-tert-butyl-1-hydroxypyrene 1 yields the exceptionally persistent and oxygen-insensitive 2,7-di-tert-butylpyren-1-oxyl radical 2 whose EPR and ENDOR spectra give the following proton hyperfine coupling (hfc) consts.: 0.526, 0.445, 0.426, 0.386, 0.157, 0.107, 0.088 and 0.0054 mT (g = 2.0037). The assignments of the protons are accomplished by measuring the EPR and ENDOR spectra of partly deuterated 2,7-di-tert-butyl(4,5,9,10-2H4)pyren-1-oxyl radical. Radical 2 is isolated as a dimer which is in equil. with 2 in soln., even at low temps. The thermodyn. parameters for the equil. are detd. to be 7.2 ± 2.0 kJ mol⁻¹ (ΔH) and -35 ± 15 J mol⁻¹ K⁻¹ (ΔS), resp. The very low ΔH and neg. ΔS values are briefly discussed.

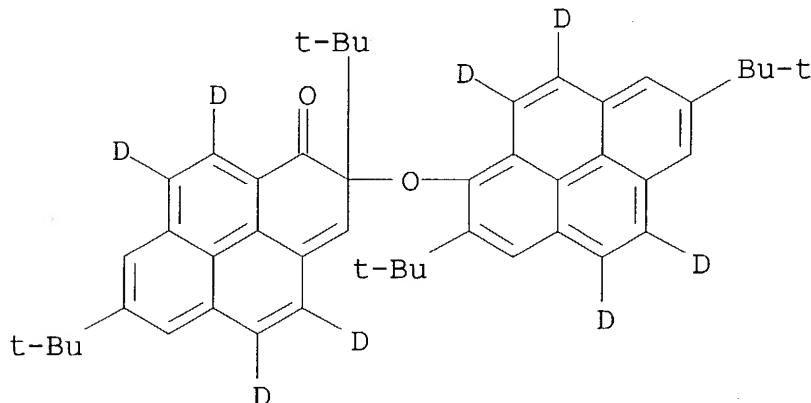
IT 176039-06-8P 176039-08-0P 176039-10-4P

176039-12-6P

(prepn., dimerization, EPR, and ENDOR of exceptionally persistent and oxygen-insensitive 2,7-di-tert-butylpyren-1-oxyl radical)

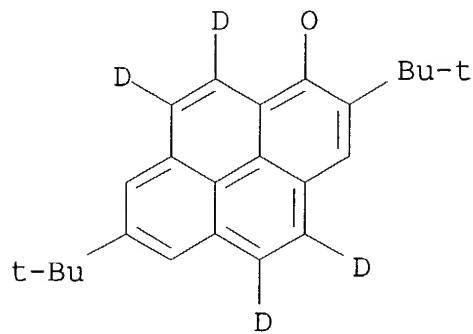
RN 176039-06-8 HCA

CN 1(2H)-Pyrenone-4,5,9,10-d4, 2-[[2,7-bis(1,1-dimethylethyl)-1-pyrenyl-4,5,9,10-d4]oxy]-2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



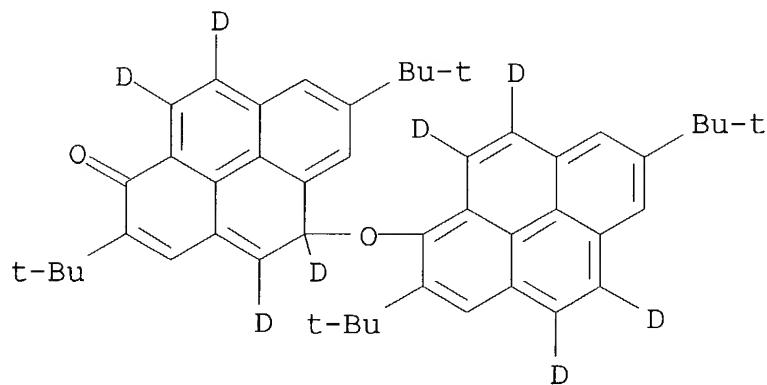
RN 176039-08-0 HCA

CN 1-Pyrenyl-4,5,9,10-d4-oxy, 2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



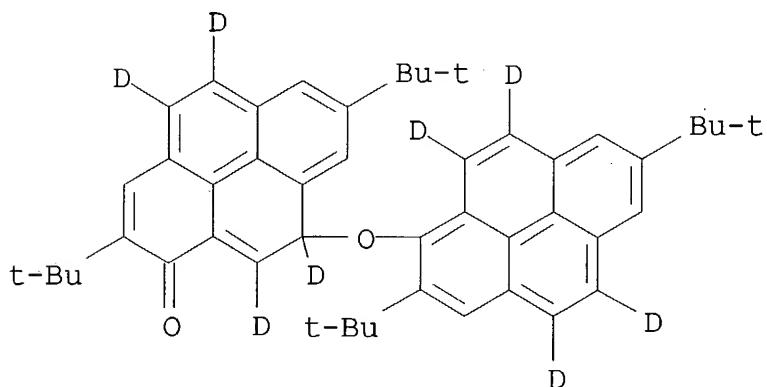
RN 176039-10-4 HCA

CN 1(5H)-Pyrenone-4,5,9,10-d4, 5-[[2,7-bis(1,1-dimethylethyl)-1-pyrenyl-4,5,9,10-d4]oxy]-2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



RN 176039-12-6 HCA

CN 1(9H)-Pyrenone-4,5,9,10-d4, 9-[[2,7-bis(1,1-dimethylethyl)-1-pyrenyl-4,5,9,10-d4]oxy]-2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

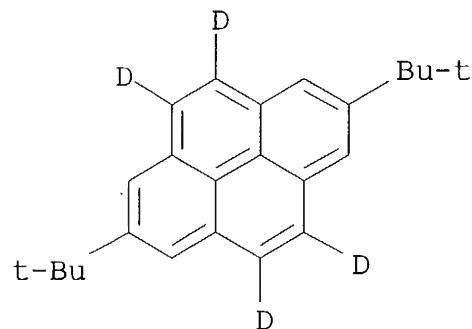


IT 160566-80-3P 176039-02-4P 176039-03-5P
 176039-04-6P

(prepn., dimerization, EPR, and ENDOR of exceptionally persistent and oxygen-insensitive 2,7-di-tert-butylpyren-1-oxyl radical)

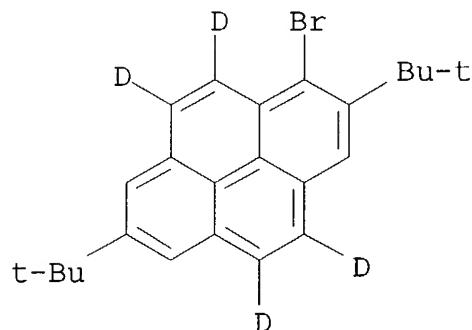
RN 160566-80-3 HCA

CN Pyrene-4,5,9,10-d4, 2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



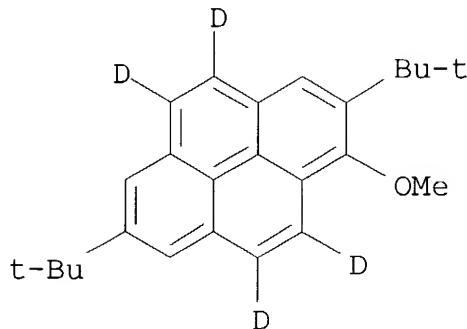
RN 176039-02-4 HCA

CN Pyrene-4,5,9,10-d4, 1-bromo-2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



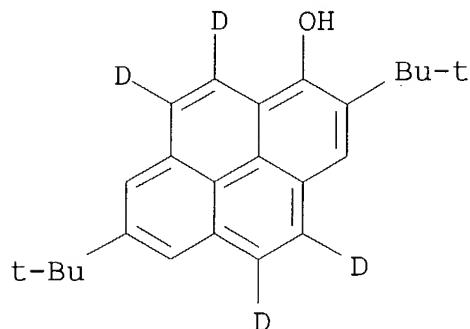
RN 176039-03-5 HCA

CN Pyrene-4,5,9,10-d4, 2,7-bis(1,1-dimethylethyl)-1-methoxy- (9CI) (CA INDEX NAME)



RN 176039-04-6 HCA

CN 1-Pyren-4,5,9,10-d4-ol, 2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



IT 176039-06-8P 176039-08-0P 176039-10-4P

176039-12-6P

(prepn., dimerization, EPR, and ENDOR of exceptionally persistent and oxygen-insensitive 2,7-di-tert-butylpyren-1-oxyl radical)

IT 160566-80-3P 176039-02-4P 176039-03-5P

176039-04-6P

(prepn., dimerization, EPR, and ENDOR of exceptionally persistent and oxygen-insensitive 2,7-di-tert-butylpyren-1-oxyl radical)

L24 ANSWER 5 OF 11 HCA COPYRIGHT 2004 ACS on STN

123:256038 ESR studies of nitrogen-centered free radicals. 47.

Generation, isolation, ESR and ^1H ENDOR spectra, and magnetic characterization of N-[(4-nitrophenyl)thio]-2-t-butyl-1-pyrenylaminyl. Miura, Yozo; Oka, Hiroyuki; Yamano, Eiji; Teki, Yoshio; Takui, Takeji; Itoh, Koichi (Faculty Engineering, Osaka City University, Osaka, 558, Japan). Bulletin of the Chemical Society of Japan, 68(4), 1187-92 (English) 1995. CODEN: BCSJA8. ISSN: 0009-2673. Publisher: Nippon Kagakkai.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

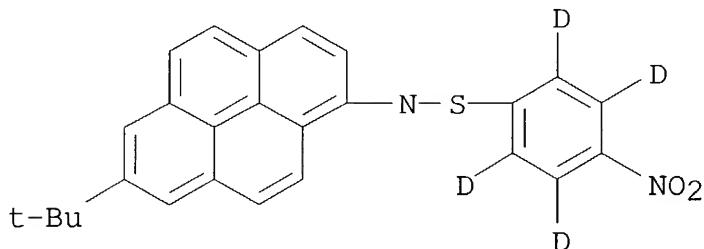
AB The oxidn. of N-[(4-nitrophenyl)thio]-2-tert-butyl-1-aminopyrene gave a persistent and oxygen-insensitive N-[(4-nitrophenyl)thio]-2-tert-butyl-1-pyrenylamino radical (I), which was isolated as reddish-black fine needles. The hyperfine coupling (hfc) consts. for the aminyl I were detd. by ESR and 1H ENDOR measurements, indicating that there is an extensive delocalization of the unpaired electron from the nitrogen onto the pyrene ring. A comparison of the hfc consts. with structurally close N-[(4-nitrophenyl)thio]-7-tert-butyl-1-pyrenylaminy (II) and N-[(4-nitrophenyl)thio]-2,7-di-tert-butyl-1-pyrenylaminy (III) showed that although the spin-d. distribution of I is similar to that of III, it is greatly different from that of II. Magnetic susceptibility measurements of I in solid radical crystals showed that the magnetic interaction between the radical spins as strongly antiferromagnetic, giving $J/k = -108$ and -192 K for III and I, resp.

IT 156268-42-7

(ESR and ENDOR of N-[(4-nitrophenyl)thio]pyrenamine radical)

RN 156268-42-7 HCA

CN Amidogen, [7-(1,1-dimethylethyl)-1-pyrenyl][(4-nitrophenyl-2,3,5,6-d4)thio]- (9CI) (CA INDEX NAME)



IT 156268-42-7

(ESR and ENDOR of N-[(4-nitrophenyl)thio]pyrenamine radical)

L24 ANSWER 6 OF 11 HCA COPYRIGHT 2004 ACS on STN

122:186798 Formation of $M+\bullet$ ions under matrix fast atom bombardment conditions: does charge exchange reaction occur?. Takayama, Mitsuo; Iwamura, Michiko; Fuchibe, Shohaku (Fac. Pharm. Sci., Toho Univ., Chiba, 274, Japan). Organic Mass Spectrometry, 29(11), 601-6 (English) 1994. CODEN: ORMSBG. ISSN: 0030-493X. Publisher: Wiley.

AB The formation of mol. ions, $M+\bullet$, under fast atom bombardment (FAB) conditions using a liq. matrix was examd. by using compds. in

which preferential $M+\bullet$ peaks appear in their FAB spectra. The FAB spectra were compared with the corresponding mass spectra obtained by electron impact (EI) ionization, chem. ionization (CI), and charge-exchange ionization (CEI) methods. All of the spectra showed preferential peaks of the $M+\bullet$ ion and a characteristic intense fragment ion peak originating from a β -fission. The FAB spectra were similar in the fragment ions appearing in the EI spectra and were very similar in the fragmentation pattern to the CEI spectra using $Ar+\bullet$ and $Xe+\bullet$ as the reagent ions. Further, the FAB spectra did not show any doubly charged ion peaks, while the 70 eV EI spectra showed the peaks of doubly charged mol. and/or fragment ions. The isobutane CI spectra of the synthesized compds. suggested that the formation of $M+\bullet$ ions occurred through the CE reaction with isobutane ion, $C_4H_{10}+\bullet$, and the CI spectra showed a marked intense fragment ion peak originating from the β -fission which seemed to occur characteristically in CEI processes. The results obtained suggested that the formation of $M+\bullet$ ions under matrix FAB conditions occurred mainly by CE reactions between the analytes M and matrix mol. ions $B+\bullet$ and/or fragment ions $b+\bullet$.

IT

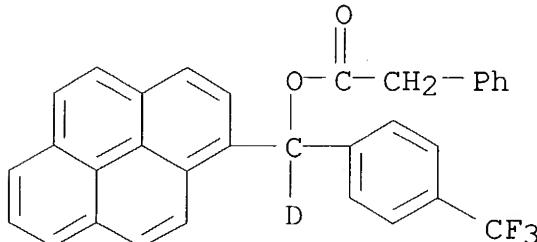
161618-41-3P(charge exchange reaction in formation of $M+\bullet$ ions under matrix fast atom bombardment conditions)

RN

161618-41-3 HCA

CN

Benzeneacetic acid, 1-pyrenyl[4-(trifluoromethyl)phenyl]methyl-d ester (9CI) (CA INDEX NAME)



IT

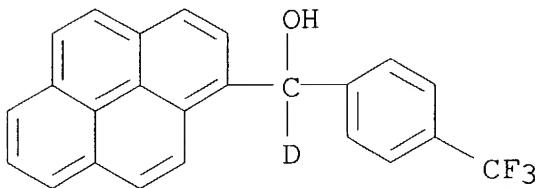
161618-45-7P(charge exchange reaction in formation of $M+\bullet$ ions under matrix fast atom bombardment conditions)

RN

161618-45-7 HCA

CN

1-Pyrenemethan- α -d-ol, α -[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



IT 161618-41-3P

(charge exchange reaction in formation of M+• ions under matrix fast atom bombardment conditions)

IT 161618-45-7P

(charge exchange reaction in formation of M+• ions under matrix fast atom bombardment conditions)

L24 ANSWER 7 OF 11 HCA COPYRIGHT 2004 ACS on STN

122:132442 ESR and 1H ENDOR Spectra of Partly Deuterated

N-[(4-Nitrophenyl)thio]-2,7-di-tert-butyl-1-pyrenylaminyl Radical.

Assignments of the Pyrene Ring Protons. Miura, Yozo; Yamano, Eiji

(Faculty of Engineering, Osaka City University, Osaka, 558, Japan).

Journal of Organic Chemistry, 60(4), 1070-3 (English) 1995. CODEN:

JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 122:132442.

Publisher: American Chemical Society.

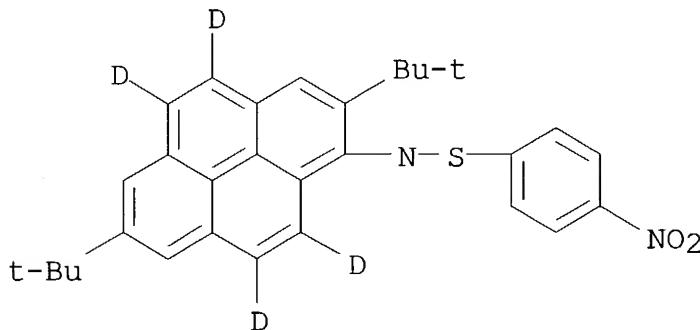
AB Partly deuterated N-[(4-nitrophenyl)thio]-2,7-di-tert-butyl-1-pyrenylaminyl-4,5,9,10-d4 radical (3) was generated and its ESR and 1H ENDOR spectra were measured. From the spectral results the proton hyperfine consts. for 3 and corresponding nondeuterated aminyl were assigned.

IT 160566-83-6P

(ESR and 1H ENDOR spectra of partly deuterated (nitrophenylthio)dibutylpyrenylaminyl radical)

RN 160566-83-6 HCA

CN Amidogen, [2,7-bis(1,1-dimethylethyl)-1-pyrenyl-4,5,9,10-d4][(4-nitrophenyl)thio]- (9CI) (CA INDEX NAME)

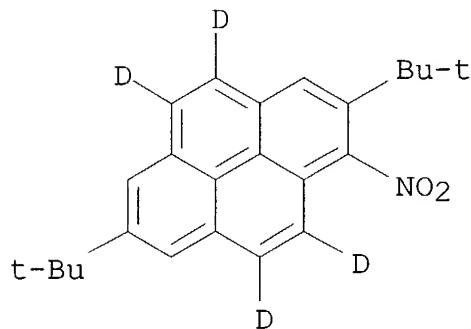


IT 160566-79-0P 160566-80-3P 160566-81-4P
 160566-82-5P

(ESR and 1H ENDOR spectra of partly deuterated
 (nitrophenylthio)dibutylpyrenylaminyl radical)

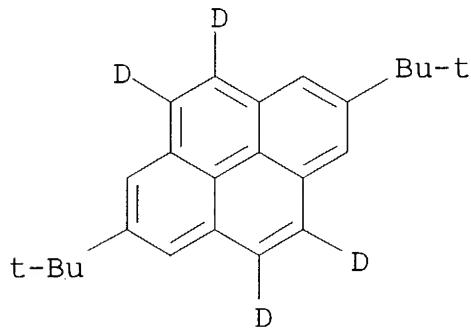
RN 160566-79-0 HCA

CN Pyrene-4,5,9,10-d4, 2,7-bis(1,1-dimethylethyl)-1-nitro- (9CI) (CA
 INDEX NAME)



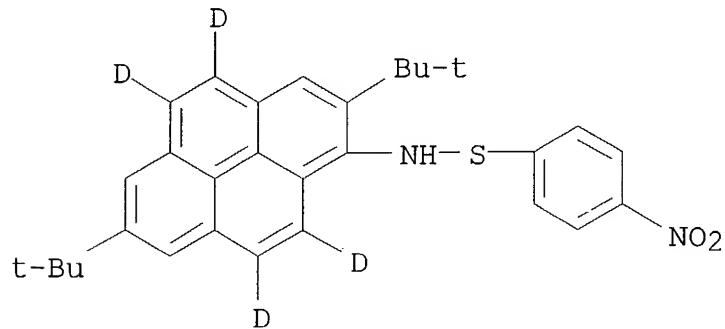
RN 160566-80-3 HCA

CN Pyrene-4,5,9,10-d4, 2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX
 NAME)



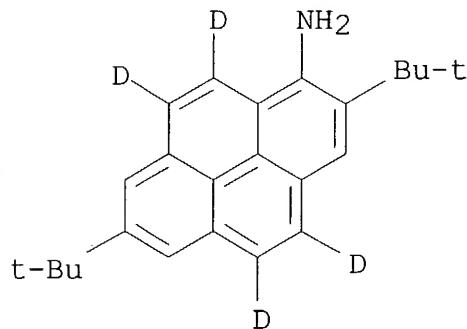
RN 160566-81-4 HCA

CN Benzenesulfenamide, N-[2,7-bis(1,1-dimethylethyl)-1-pyrenyl-4,5,9,10-d4]-4-nitro- (9CI) (CA INDEX NAME)



RN 160566-82-5 HCA

CN 1-Pyren-4,5,9,10-d4-amine, 2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



IT 160566-83-6P

(ESR and 1H ENDOR spectra of partly deuterated (nitrophenylthio)dibutylpyrenylaminyl radical)

IT 160566-79-0P 160566-80-3P 160566-81-4P

160566-82-5P

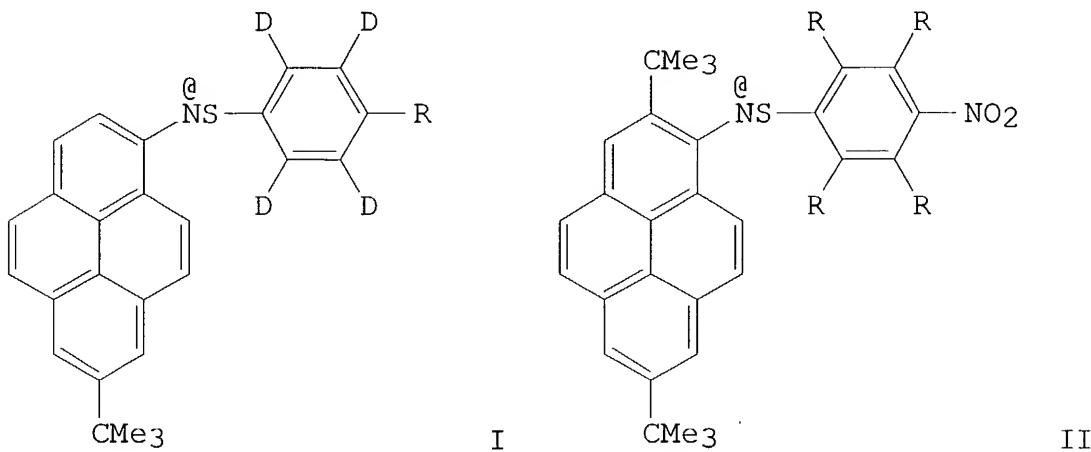
(ESR and 1H ENDOR spectra of partly deuterated (nitrophenylthio)dibutylpyrenylaminyl radical)

L24 ANSWER 8 OF 11 HCA COPYRIGHT 2004 ACS on STN

121:82367 Generation, Isolation, and Characterization of

N-(Arylthio)-7-tert-butyl- and N-(Arylthio)-2,7-di-tert-butyl-1-pyrenylaminyl Radicals. Miura, Yozo; Yamano, Eiji; Tanaka, Akio; Yamauchi, Jun (Faculty of Engineering, Osaka City University, Osaka, 558, Japan). Journal of Organic Chemistry, 59(12), 3294-300 (English) 1994. CODEN: JOCEAH. ISSN: 0022-3263.

GI



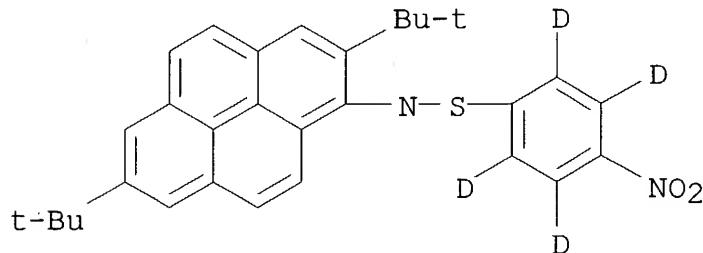
AB N-(Arylthio)-7-tert-butyl-1-pyrenylaminyl (I; R = D, Br, NO₂) and N-[(4-nitrophenyl)thio]-2,7-di-tert-butyl-1-pyrenylaminyl radicals (II; R = H, D) are prep'd. by PbO₂ oxidn. of the corresponding amines and studied by ESR and ENDOR spectroscopy. The kinetic ESR study shows that, while I gradually decomp. in soln. at room temp., II is quite persistent, even in refluxing benzene, and shows no tendency to dimerize, even at low temps. These interesting properties of II permit the isolation of II as radical crystals in 28-31% yield. The hyperfine splitting (hfs) consts. of I and II, detd. by ESR and ENDOR spectroscopic methods, show an extensive delocalization of the unpaired electron onto the pyrene ring. Comparison of the hfs consts. of I and II shows that a more extensive delocalization of the spin into the pyrene ring takes place in II. This is accounted for in terms of the difference in the conformations of I and II.

IT 144614-52-8P

(formation and ESR and ENDOR of)

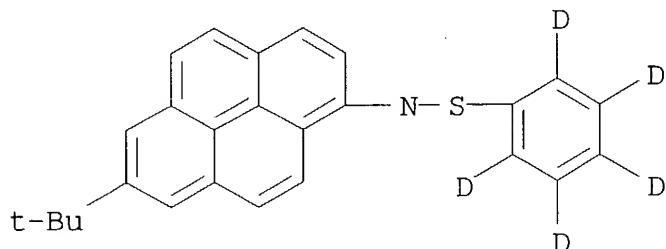
RN 144614-52-8 HCA

CN Amidogen, [2,7-bis(1,1-dimethylethyl)-1-pyrenyl][(4-nitrophenyl-2,3,5,6-d4)thio]-(9CI) (CA INDEX NAME)

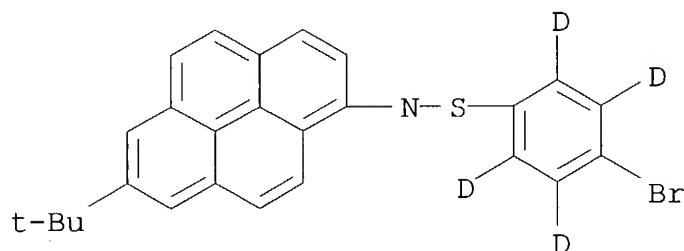


IT 156268-40-5P 156268-41-6P 156268-42-7P

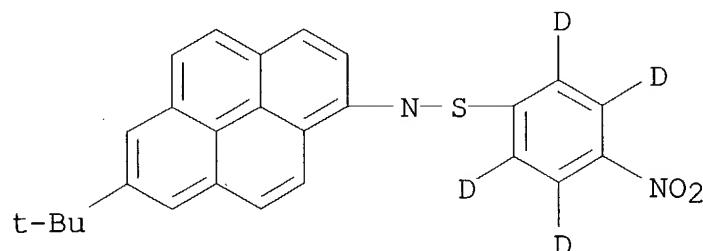
RN (formation and ESR of)
 156268-40-5 HCA
 CN Amidogen, [7-(1,1-dimethylethyl)-1-pyrenyl](phenyl-d5-thio)- (9CI)
 (CA INDEX NAME)



RN 156268-41-6 HCA
 CN Amidogen, [(4-bromophenyl-2,3,5,6-d4)thio][7-(1,1-dimethylethyl)-1-pyrenyl]- (9CI) (CA INDEX NAME)

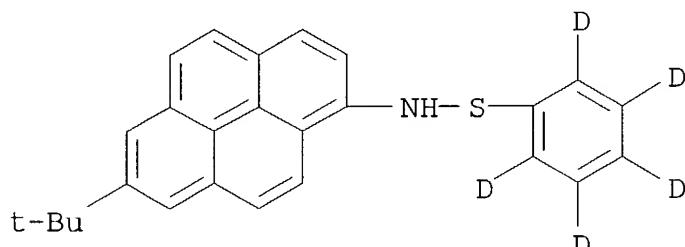


RN 156268-42-7 HCA
 CN Amidogen, [7-(1,1-dimethylethyl)-1-pyrenyl][(4-nitrophenyl-2,3,5,6-d4)thio]- (9CI) (CA INDEX NAME)



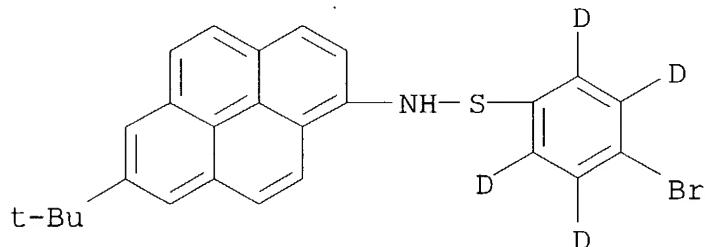
IT 156268-45-0P 156268-47-2P 156268-49-4P
 (prepn. and oxidn. to radical)

RN 156268-45-0 HCA
 CN Benzene-d5-sulfenamide, N-[7-(1,1-dimethylethyl)-1-pyrenyl]- (9CI)
 (CA INDEX NAME)



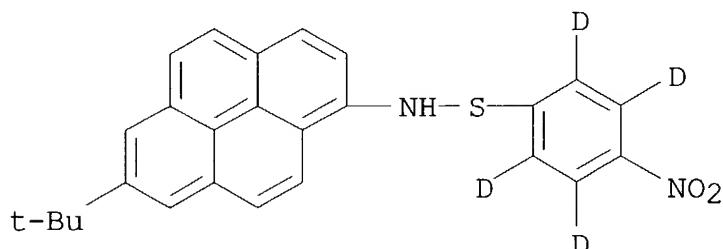
RN 156268-47-2 HCA

CN Benzene-2,4,5,6-d4-sulfenamide, 4-bromo-N-[7-(1,1-dimethylethyl)-1-pyrenyl]- (9CI) (CA INDEX NAME)



RN 156268-49-4 HCA

CN Benzene-2,4,5,6-d4-sulfenamide, N-[7-(1,1-dimethylethyl)-1-pyrenyl]-4-nitro- (9CI) (CA INDEX NAME)



IT 144614-52-8P

(formation and ESR and ENDOR of)

IT 156268-40-5P 156268-41-6P 156268-42-7P

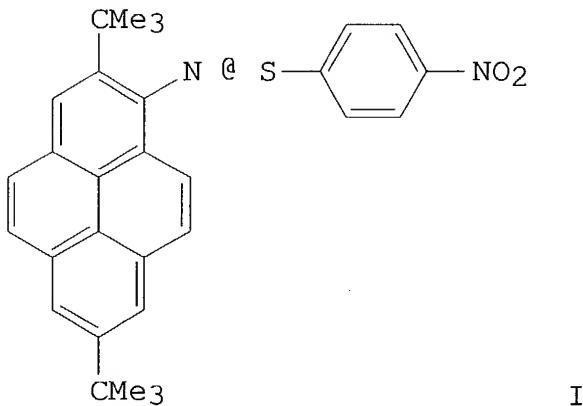
(formation and ESR of)

IT 156268-45-0P 156268-47-2P 156268-49-4P

(prepn. and oxidn. to radical)

Preparation and isolation of an exceptionally persistent nitrogen-centered free radical. N-[(4-nitrophenyl)thio]-2,7-di-t-butyl-1-pyrenylaminyl. Miura, Yozo; Yamano, Eiji; Tanaka, Akio; Ogo, Yoshiaki (Fac. Eng., Osaka City Univ., Osaka, 558, Japan). Chemistry Letters (9), 1831-4 (English) 1992. CODEN: CMLTAG. ISSN: 0366-7022. OTHER SOURCES: CASREACT 117:250875.

GI



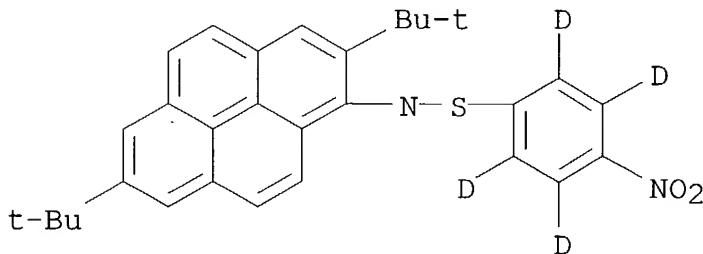
AB The title persistent, oxygen-insensitive radical I was prep'd. as pure radical crystals in 31% yield by oxidn. of its amino precursor with PbO2. The ESR spectrum of I is reported. The crystals can be stored, without decompn., for a long period.

IT **144614-52-8**

(ESR of)

RN 144614-52-8 HCA

CN Amidogen, [2,7-bis(1,1-dimethylethyl)-1-pyrenyl][(4-nitrophenyl-2,3,5,6-d4)thio]- (9CI) (CA INDEX NAME)

IT **144614-52-8**

(ESR of)

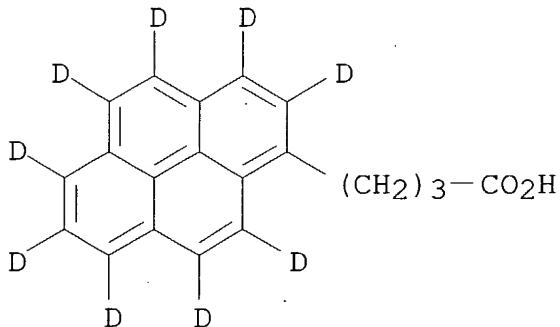
L24 ANSWER 10 OF 11 HCA COPYRIGHT 2004 ACS on STN
 116:249957 Superoxide chemical transformation of diolepoxyde
 polyaromatic hydrocarbon DNA adducts. Determination of
 benzo[a]pyrene-r-7,t-8,9,c-10-tetrahydrotetrol by gas
 chromatography. Li, Wenni; Sotiriou-Leventis, Chariklia;
 Abdel-Baky, Samy; Fisher, Daniel H.; Giese, Roger W. (Coll. Pharm.
 Allied Health Professions, Northeastern Univ., Boston, MA, 02115,
 USA). Journal of Chromatography, 588(1-2), 273-80 (English) 1991.
 CODEN: JOCRAM. ISSN: 0021-9673.

AB Benzo[a]pyrene-r-7,t-8,9,c-10-tetrahydrotetrol (100 pg, 342 fmol)
 was measured using the following sequence of steps: (1) chem.
 transformation with potassium superoxide to 2,3-pyrenedicarboxylic
 acid; (2) electrophore derivatization with pentafluorobenzyl
 bromide; (3) sample clean-up by high-performance liq. chromatog. and
 (4) measurement by gas chromatog. with electron-capture detection
 and by gas chromatog. with electron-capture neg.-ion mass
 spectrometry. The overall, abs. yields obtained by the two
 procedures were 69% and 60%, resp. This work completes the first
 stage towards the establishment of a general method for detecting
 diolepoxyde polyarom. hydrocarbon DNA adducts by gas chromatog.

IT 139623-28-2P
 (prepn. and dihydrobenzopyrenone prepn. from)

RN 139623-28-2 HCA

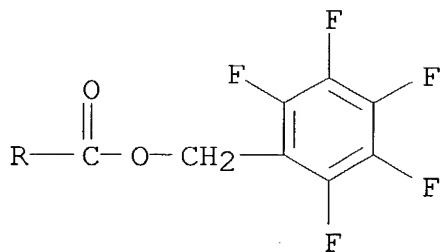
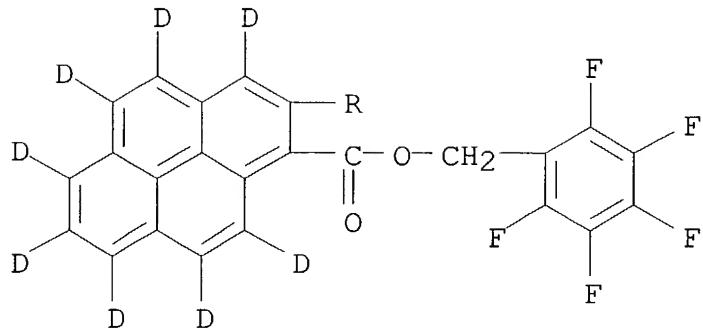
CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d9-butanoic acid (9CI) (CA INDEX NAME)



IT 139623-29-3P
 (prepn. and oxidn. and pentafluorobenzyl deriv. prepn. from)

RN 139623-29-3 HCA

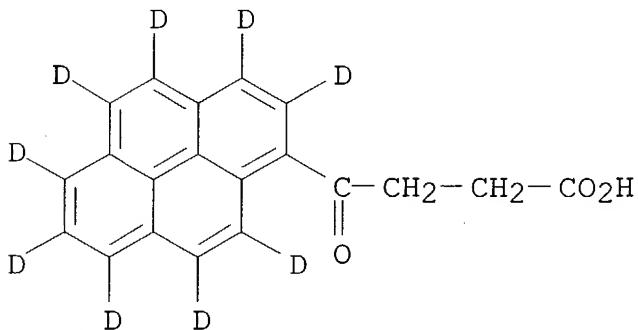
CN 1,2-Pyrene-3,4,5,6,7,8,9,10-d8-dicarboxylic acid,
 bis[(pentafluorophenyl)methyl] ester (9CI) (CA INDEX NAME)



IT 139649-53-9P

(prepn. and redn. of)

RN 139649-53-9 HCA

CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d9-butanoic acid, γ -oxo-, sodium salt (9CI) (CA INDEX NAME)

● Na

IT 139623-28-2P

(prepn. and dihydrobenzopyrenone prepн. from)

IT 139623-29-3P

(prepn. and oxidn. and pentafluorobenzyl deriv. prepn. from)
 IT 139649-53-9P
 (prepn. and redn. of)

L24 ANSWER 11 OF 11 HCA COPYRIGHT 2004 ACS on STN
 97:103053 Deuteron NMR line shapes and molecular motion in solid
 charge-transfer complexes. Ripmeester, J. A. (Div. Chem., Natl.
 Res. Counc. Canada, Ottawa, ON, K1A 0R9, Can.). Journal of Chemical
 Physics, 77(2), 1069-70 (English) 1982. CODEN: JCPSA6. ISSN:
 0021-9606.

AB D NMR line shapes were obtained for naphthalene-d8-TCNB,
 naphthalene-d8-TCNE, pyrene-d10, and pyrene-d10-dinitrochlorobenzene
 at 27.63 MHz. The results are interpreted in terms of a dynamic
 model, and quadrupole coupling consts. and asymmetry parameters are
 obtained.

IT 82748-83-2
 (NMR of)

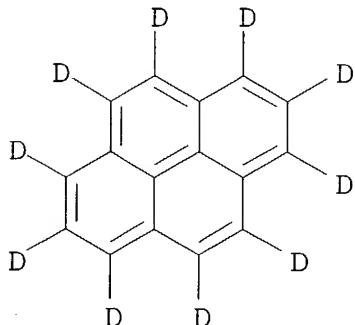
RN 82748-83-2 HCA

CN Pyrene-d10, compd. with 1-chloro-2,4-dinitrobenzene (1:1) (9CI) (CA
 INDEX NAME)

CM 1

CRN 1718-52-1

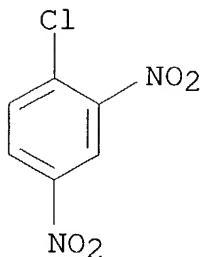
CMF C16 D10



CM 2

CRN 97-00-7

CMF C6 H3 Cl N2 O4



IT 82748-83-2
(NMR of)

=> d 125 1-28 cbib abs hitstr hitrn

L25 ANSWER 1 OF 28 HCA COPYRIGHT 2004 ACS on STN

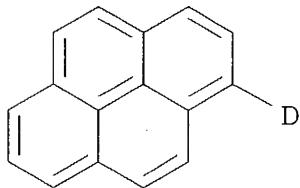
139:291888 Possible molecular hydrogen formation mediated by the radical cations of anthracene and pyrene. Hirama, Mutsumi; Ishida, Toshimasa; Aihara, Jun-Ichi (Department of Chemistry, Faculty of Science, Shizuoka University Oya, Shizuoka, 422-8529, Japan). Journal of Computational Chemistry, 24(12), 1378-1382 (English) 2003. CODEN: JCCHDD. ISSN: 0192-8651. Publisher: John Wiley & Sons, Inc..

AB H mols. cannot be formed readily by the assocn. of gaseous H atoms. Possible H₂ formation mediated by the radical cations of typical polycyclic arom. hydrocarbons (PAHs), anthracene and pyrene, was studied at the B3LYP/6-31G** level of theory. The authors presumed that H₂ is formed by way of two elementary reactions: the addn. of an H atom to a PAH mol. cation, and the H abstraction from the resulting monohydro-PAH cation (i.e., arenium ion) by a second H atom to yield H₂. The first reaction takes place without any activation energy. The second reaction is also predicted to proceed along almost barrierless pathways, although it is far from being a typical ion-mol. reaction. There is a possibility that these reactions might constitute one of the mechanisms for H₂ formation in extremely cold interstellar space. D enrichment in PAH cations is possibly accompanied by such H₂ formation because deuteration lowers the energies of polyat. PAH cations appreciably.

IT 608135-13-3
(mol. hydrogen formation mediated by radical cations of anthracene and pyrene)

RN 608135-13-3 HCA

CN Pyrene-1-d, radical ion(1+) (9CI) (CA INDEX NAME)



IT 608135-13-3

(mol. hydrogen formation mediated by radical cations of anthracene and pyrene)

L25 ANSWER 2 OF 28 HCA COPYRIGHT 2004 ACS on STN

139:276611 Real-time observation of bimodal proton transfer in acid-base pairs in water. Rini, Matteo; Magnes, Ben-Zion; Pines, Ehud; Nibbering, Erik T. J. (Max Born Institut fuer Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, D-12489, Germany). Science (Washington, DC, United States), 301(5631), 349-352 (English) 2003. CODEN: SCIEAS. ISSN: 0036-8075. Publisher: American Association for the Advancement of Science.

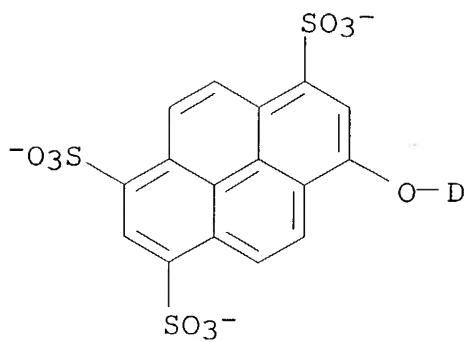
AB The neutralization reaction between an acid and a base in water, triggered after optical excitation, was studied by femtosecond vibrational spectroscopy. Bimodal dynamics were obsd. In H-bonded acid-base complexes, the proton transfer proceeds extremely fast (within 150 fs). In encounter pairs formed by diffusion of uncomplexed photoacid and base mols., the reaction upon contact was an order of magnitude slower, in agreement with earlier reported values. These results call for a refinement of the traditional Eigen-Weller picture of acid-base reactions: A three-stage model is introduced to account for all obsd. dynamics.

IT 604766-94-1

(real-time observation of bimodal proton transfer in acid-base pairs in water)

RN 604766-94-1 HCA

CN 1,3,6-Pyrenetrisulfonic acid, 8-(hydroxy-d)-, ion(3-) (9CI) (CA INDEX NAME)



IT 604766-94-1

(real-time observation of bimodal proton transfer in acid-base pairs in water)

L25 ANSWER 3 OF 28 HCA COPYRIGHT 2004 ACS on STN

138:38974 N-tert-Butoxy-1-aminopyrenyl Radicals. Isolation, Electronic Structure, and Magnetic Characterization. Miura, Yozo; Matsuba, Nobuaki; Tanaka, Rika; Teki, Yoshio; Takui, Takeji (Graduate School of Engineering, Department of Applied Chemistry, Osaka City University, Sumiyoshi-ku, Osaka, 558-8585, Japan). Journal of Organic Chemistry, 67(25), 8764-8770 (English) 2002. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 138:38974. Publisher: American Chemical Society.

AB N-tert-Butoxy-2,7-di-tert-butyl-1-pyrenylaminy (4), N-tert-butoxy-2-tert-butyl-1-pyrenylaminy (5), and N-tert-butoxy-7-tert-butyl-1-pyrenylaminy (6) free radicals were generated by the reaction of the lithium amides of the corresponding 1-aminopyrenes with tert-Bu peroxybenzoate in THF at -78 °C. Although 6 could not be isolated due to the gradual decompn. in soln., 4 and 5 were quite persistent and could be isolated as monomeric radical crystals. The X-ray crystallog. analyses for the isolated free radicals were successfully carried out, indicating that the N and O atoms are almost coplanar with the pyrene ring. The ESR spectra of 4 and 5 were very complex due to the presence of many magnetically unequivalent protons. Therefore, the proton hyperfine coupling (hfc) consts. were detd. by 1H ENDOR/TRIPLE resonance spectroscopy. To assign the hfc consts. for the pyrene ring protons, a partially deuterated radical, 4-d4, was prep'd. and the ENDOR and ESR spectra were measured. To discuss the spin d. distribution for 4 and 5 ab initio MO calcns. were performed by the DFT UBecke 3LYP method, using the STO 6-31G basis set. Magnetic susceptibility measurements were carried out for 4 and 5 with a SQUID magnetometer. For 4 a weak antiferromagnetic interaction was obsd., and for 5 a very strong antiferromagnetic interaction was obsd. The antiferromagnetic interactions were explained by their

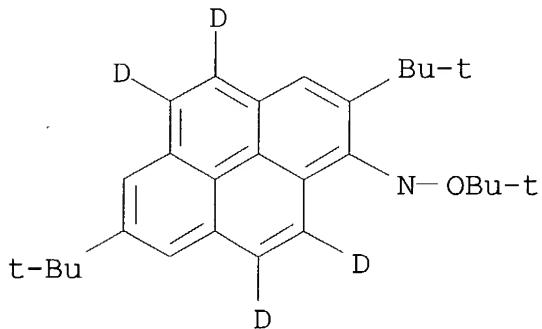
crystal structures.

IT **478921-79-8P**

(isolation, crystallog. and electronic structure, and magnetic characterization of N-tert-butoxy-1-aminopyrenyl radicals)

RN 478921-79-8 HCA

CN Amidogen, [2, 7-bis(1,1-dimethylethyl)-1-pyrenyl-4,5,9,10-d4] (1,1-dimethylethoxy)- (9CI) (CA INDEX NAME)

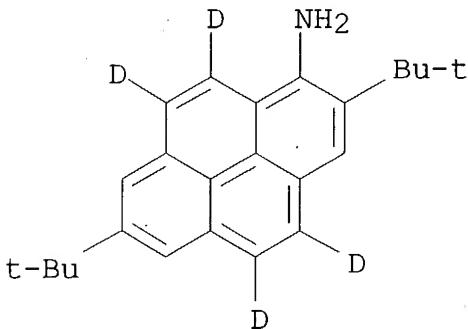


IT **160566-82-5**

(lithiation/N-tert-butoxylation; isolation, crystallog. and electronic structure, and magnetic characterization of N-tert-butoxy-1-aminopyrenyl radicals)

RN 160566-82-5 HCA

CN 1-Pyren-4,5,9,10-d4-amine, 2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



IT **478921-79-8P**

(isolation, crystallog. and electronic structure, and magnetic characterization of N-tert-butoxy-1-aminopyrenyl radicals)

IT **160566-82-5**

(lithiation/N-tert-butoxylation; isolation, crystallog. and electronic structure, and magnetic characterization of N-tert-butoxy-1-aminopyrenyl radicals)

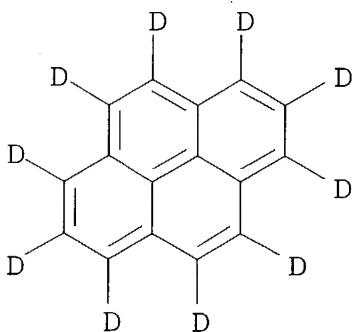
L25 ANSWER 4 OF 28 HCA COPYRIGHT 2004 ACS on STN
 137:325127 Electron Localization in Liquid Acetonitrile. Shkrob, I. A.;
 Sauer, M. C., Jr. (Chemistry Division, Argonne National Laboratory,
 Argonne, IL, 60439, USA). Journal of Physical Chemistry A, 106(39),
 9120-9131 (English) 2002. CODEN: JPCAFH. ISSN: 1089-5639.
 Publisher: American Chemical Society.

AB Time-resolved one- and two-pulse laser dc photocond. has been used to observe two kinds of reducing species, anion-1 and anion-2, in liq. acetonitrile. At 25 °C, the std. enthalpy of conversion from anion-1 to anion-2 is -44.3 ± 3.6 kJ/mol and the conversion time is .apprx.3 ns. The high-temp. form, anion-1, absorbs in the IR and migrates >3.3 times faster than any other ion in acetonitrile. This rapid migration has a low activation energy of 3.2 kJ/mol (vs .apprx.7.6 kJ/mol for other ions). Anion-1 rapidly transfers the electron to acceptors with high electron affinity, with rate const. up to $1011 \text{ M}^{-1} \text{ s}^{-1}$. The low-temp. form, anion-2, absorbs in the visible and exhibits normal mobility and electron-transfer rates, ca. $1.5 + 1010 \text{ M}^{-1} \text{ s}^{-1}$. It reacts, by proton transfer, with two hydrogen-bonded mols. of water and/or aliph. alcs. Laser photoexcitation of these two solvent anions in their resp. absorption bands leads to the formation of CH_3 and CN^- . We present arguments indicating that anion-2 is a dimer radical anion of acetonitrile, whereas anion-1 is a multimer radical anion that may be regarded as a "solvated electron".

IT 159169-39-8, Pyrene-d10, radical ion(1+)
 (ESR and photocond. study on electron localization in liq.
 acetonitrile)

RN 159169-39-8 HCA

CN Pyrene-d10, radical ion(1+) (9CI) (CA INDEX NAME)



IT 159169-39-8, Pyrene-d10, radical ion(1+)
 (ESR and photocond. study on electron localization in liq.
 acetonitrile)

L25 ANSWER 5 OF 28 HCA COPYRIGHT 2004 ACS on STN

137:140349 Preparation of homochiral aromatic compounds as chiral

solvating agents and chiral auxiliaries. Virgili Moya, Albert (Universitat Autonoma de Barcelona, Spain). Span. ES 2160464 A1 20011101, 16 pp. (Spanish). CODEN: SPXXAD. APPLICATION: ES 1998-2628 19981209.

AB Homochiral compds. X-A-CR1R2R3 [A represents a deuterated arom. or heteroarom. ring system (1-6 rings); X = D, halo, an electrophilic group such as NO₂ or an electron donor group such as OR' or NR'R'', where R' and R'' = alkyl, aryl, acyl, D or H; R1 = H or D; R2 = OR', NR'R'''; R3 = CF₃, alkyl, aryl, or acyl which is optionally deuterated or fluorinated] were prep'd. for use as chiral solvating agents and chiral auxiliaries. These compds. do not produce a signal in ¹H NMR. Thus, (R)-perdeutero-2,2,2-trifluoro-1-(9-anthryl)ethanol (I) was prep'd. from perdeuterated anthracene by trifluoroacetylation, redn. with LiAlD₄, acetylation, resoln. by HPLC, and sapon. The ¹H NMR of (±)-1-phenyl-1,2-ethanediol carried out at 400 MHz in the presence of I showed distinct signal for each enantiomer.

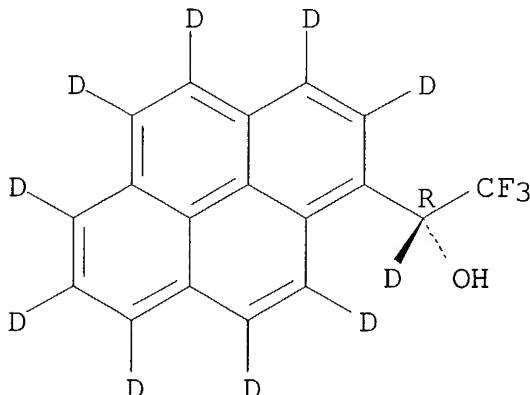
IT 295429-45-7P 295429-50-4P

(prepn. of perdeuterated homochiral arom. compds. as chiral solvating agents and chiral auxiliaries)

RN 295429-45-7 HCA

CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d₉-methan- α -d-ol,
 α -(trifluoromethyl)-, (α R)- (9CI) (CA INDEX NAME)

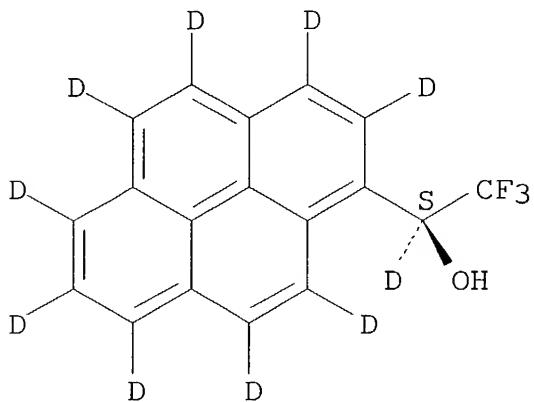
Absolute stereochemistry. Rotation (-).



RN 295429-50-4 HCA

CN 1-Pyrene-2,3,4,5,6,7,8,9,10-d₉-methan- α -d-ol,
 α -(trifluoromethyl)-, (α S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 295429-45-7P 295429-50-4P

(prepn. of perdeuterated homochiral arom. compds. as chiral solvating agents and chiral auxiliaries)

L25 ANSWER 6 OF 28 HCA COPYRIGHT 2004 ACS on STN

134:56399 Radiofrequency magnetic field effects on chemical reaction yields. Stass, D. V.; Woodward, J. R.; Timmel, C. R.; Hore, P. J.; McLauchlan, K. A. (Physical and Theoretical Chemistry Laboratory, Oxford University, Oxford, OX1 3QZ, UK). Chemical Physics Letters, 329(1,2), 15-22 (English) 2000. CODEN: CHPLBC. ISSN: 0009-2614. Publisher: Elsevier Science B.V..

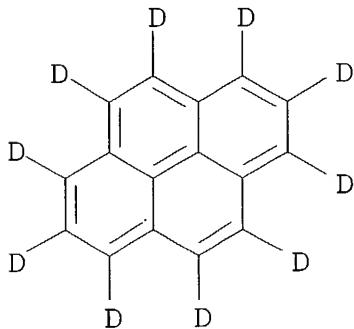
AB The influence of radiofrequency magnetic fields (1-80 MHz) on the yields of radical recombination reactions is investigated. A decrease in the recombination probability of radical ion pairs (monitored via exciplex fluorescence) is detected when the radiofrequency matches energy-level splittings arising from hyperfine interactions in the radicals. The dependence of the oscillating magnetic field effect (OMFE) spectrum on radiofrequency field strength and hyperfine coupling consts. is presented for several reaction partners. The exptl. studies are supported by theor. simulations of recombination yields based on the radical pair mechanism (RPM).

IT 127619-33-4 159169-39-8

(radiofrequency magnetic field effects on recombination yields of radical ion pairs)

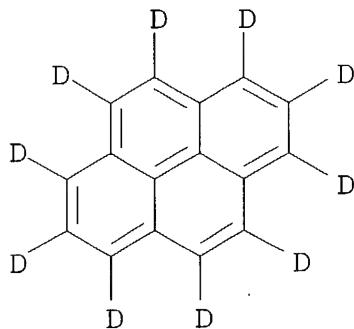
RN 127619-33-4 HCA

CN Pyrene-d10, radical ion(1-) (9CI) (CA INDEX NAME)



RN 159169-39-8 HCA

CN Pyrene-d10, radical ion(1+) (9CI) (CA INDEX NAME)



IT 127619-33-4 159169-39-8

(radiofrequency magnetic field effects on recombination yields of radical ion pairs)

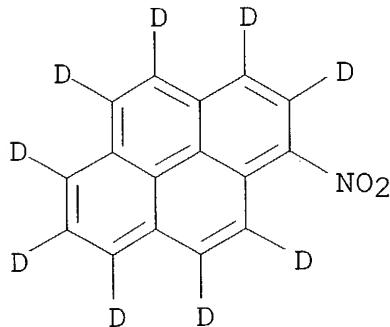
L25 ANSWER 7 OF 28 HCA COPYRIGHT 2004 ACS on STN

128:144458 Fractionation of nitro and hydroxy polynuclear aromatic hydrocarbons from extracts of air particulates by supercritical fluid chromatography. Medvedovici, Andrei; David, Frank; Desmet, Gilbert; Sandra, Pat (Department of Organic Chemistry, University of Gent, Ghent, B-9000, Belg.). Journal of Microcolumn Separations, 10(1), 89-97 (English) 1998. CODEN: JMSEEJ. ISSN: 1040-7685.
 Publisher: John Wiley & Sons, Inc..

AB Nitrated and hydroxylated polynuclear arom. hydrocarbons (nitro- and hydroxy-PAHs) extd. from air particulates were fractionated from other micropollutants by semi-preparative packed-column supercrit. fluid chromatog. on silica gel. Sample injection and fraction collection was automated by means of a Gilson 233 XL sample prep. station. The collected fractions were analyzed by capillary GC-mass spectrometry operated in the ion-monitoring mode. For some specific solutes, concns. down to the 1 pg/m³ level could be measured.

IT 93487-20-8, 1-Nitropyrene-d9
 (fractionation of nitro and hydroxy polynuclear arom.
 hydrocarbons from exts. of air particulates by supercrit. fluid
 chromatog.)

RN 93487-20-8 HCA
 CN Pyrene-1,2,3,4,5,6,7,9,10-d9, 8-nitro- (9CI) (CA INDEX NAME)



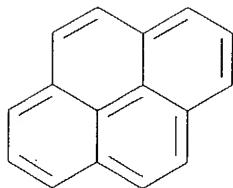
IT 93487-20-8, 1-Nitropyrene-d9
 (fractionation of nitro and hydroxy polynuclear arom.
 hydrocarbons from exts. of air particulates by supercrit. fluid
 chromatog.)

L25 ANSWER 8 OF 28 HCA COPYRIGHT 2004 ACS on STN
 126:199643 Deuterium labeling study of the gas-phase reaction of Fe+/Cr+
 with pyrene by FTMS. Srzic, Dunja; Kazazic, Sasa; Klasinc, Leo
 (Ruder Boskovic Institute, Zagreb, HR-10001, Croatia). Croatica
 Chemica Acta, 69(4), 1449-1454 (English) 1996. CODEN: CCACAA.
 ISSN: 0011-1643. Publisher: Croatian Chemical Society.

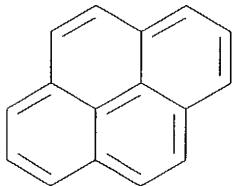
AB A .apprx. 10: 1 mixt. of deuterated with undeuterated pyrene was
 used to study the product compn. in the reaction with various ratios
 of Fe+ and Cr+ (10: 1 to 1: 10) ions in a Fourier-transform mass
 spectrometer. None of the products FePy+, CrPy+, Py+, FePy2+,
 CrPy2+ and Py2+ showed deviation from the statistically expected
 compn.

IT 187686-02-8, Pyrene-d9 187686-03-9, Pyrene-d8
 (deuterium labeling study of gas-phase reaction of iron/chromium
 cation with pyrene by FTMS)

RN 187686-02-8 HCA
 CN Pyrene-d9 (9CI) (CA INDEX NAME)



RN 187686-03-9 HCA
CN Pyrene-d8 (9CI) (CA INDEX NAME)



IT 187686-02-8, Pyrene-d9 187686-03-9, Pyrene-d8
(deuterium labeling study of gas-phase reaction of iron/chromium cation with Pyrene by FTMS)

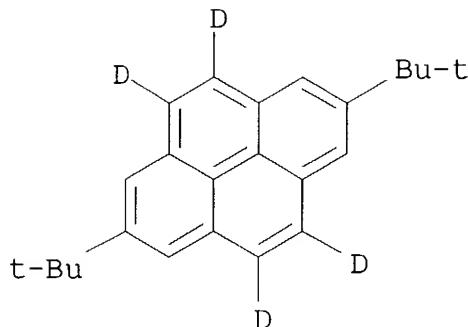
L25 ANSWER 9 OF 28 HCA COPYRIGHT 2004 ACS on STN

126:157218 Convenient Deuteriation of Bromo Aromatic Compounds by Reductive Debromination with Sodium Amalgam in CH3OD. Miura, Yozo; Oka, Hiroyuki; Yamano, Eiji; Morita, Masanori (Department of Applied Chemistry Faculty of Engineering, Osaka City University, Osaka, 558, Japan). Journal of Organic Chemistry, 62(4), 1188-1190 (English) 1997. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 126:157218. Publisher: American Chemical Society.

AB Reductive debromination of bromo arom. compds. with sodium amalgam in refluxing CH3OD gave the corresponding deuterated compds. with high isotopic purities in high yields.

IT 160566-80-3P
(deuteriation of bromo arom. compds. by reductive debromination with sodium amalgam in CH3OD)

RN 160566-80-3 HCA
CN Pyrene-4,5,9,10-d4, 2,7-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



IT 160566-80-3P

(deuteriation of bromo arom. compds. by reductive debromination with sodium amalgam in CH3OD)

L25 ANSWER 10 OF 28 HCA COPYRIGHT 2004 ACS on STN

124:260169 Relative Solution Electron Affinities of Selectively Deuteriated Pyrenes: Correlations between Voltammetric, Electron Paramagnetic Resonance, and Semiempirical PM3 Data. Hammerich, Ole; Nielsen, Merete F.; Zuilhof, Han; Mulder, Patrick P. J.; Lodder, Gerrit; Reiter, Richard C.; Kage, David E.; Rice, Charles V.; Stevenson, Cheryl D. (Department of Chemistry, University of Copenhagen, Copenhagen, DK-2100, Den.). Journal of Physical Chemistry, 100(9), 3454-62 (English) 1996. CODEN: JPCHAX. ISSN: 0022-3654. Publisher: American Chemical Society.

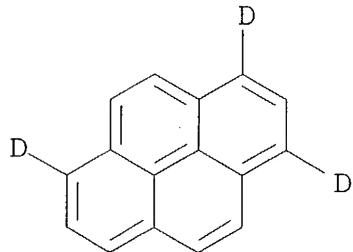
AB The equil. isotope effects (EIE) for the one-electron transfer between pyrene and seven regioselectively deuterated pyrene isotopic isomers in DMF with 0.1 M tetrabutylammonium hexafluorophosphate were measured electrochem. These data correlate linearly with the free energies (ΔG°) obtained in THF using ESR (EPR) techniques. However, the slope of the resulting line is not unity, and it indicates that the EIE in the DMF system is only two-thirds of that in the THF system. PM3 calcd. ΔG° 's, which would correspond to the gas phase electron transfers, also correlate linearly with both sets of exptl. data, but the predicted magnitudes of the EIE's are smaller than those obsd. exptl. by either technique. The nonunity slopes probably reflect slight differences in ion solvation and/or ion assocn. parameters between the anion radicals of the isotopic isomers. No general relationship between the EIE and the charge on the hydrogen/deuterium substituted carbon atom was found.

IT 167871-51-4P, Pyrene-1,3,6-d3 167871-60-5P,
 Pyrene-1,2,7-d3 167871-61-6P, Pyrene-1,2,3,4,5,6,7,8,9-d9
 169311-87-9P, Pyrene-1,4,5,9,10-d5 169311-88-0P,
 Pyrene-2,4,5,9,10-d5 174809-18-8P, Pyrene-2,4,7-d3
 174809-24-6P, Pyrene-2-d 174809-25-7P,

Pyrene-2,4,5,7,9-d5 **174809-26-8P**, Pyrene-4,5,9-d3
174809-27-9P, Pyrene-1,2,3,4,6,7,8-d7 **174809-28-0P**
, Pyrene-1,2,3,6,7-d5 **174809-29-1P**, Pyrene-1,2,3,4,6,7-d6
174809-30-4P, Pyrene-1,2,3,6,8-d5 **174809-31-5P**,
Pyrene-1,2,3,4,6,8-d6 **174809-32-6P**, Pyrene-1,2,3,4,5,6,7,8-
d8 **174809-33-7P**, Pyrene-1,2,4,5,7,9,10-d7
174809-34-8P, Pyrene-1,2,3,4,5,6,8,9,10-d9
174809-35-9P, Pyrene-1,3,4,5,6,8,9-d7 **174809-36-0P**
, Pyrene-1,3,4,5,6,9,10-d7 **174819-54-6P**, Pyrene-d4
(correlations between voltammetric, ESR, and semiempirical PM3
calcns. and relative soln. electron affinities of selectively
deuterated pyrenes)

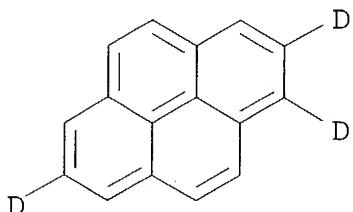
RN 167871-51-4 HCA

CN Pyrene-1,3,6-d3 (9CI) (CA INDEX NAME)



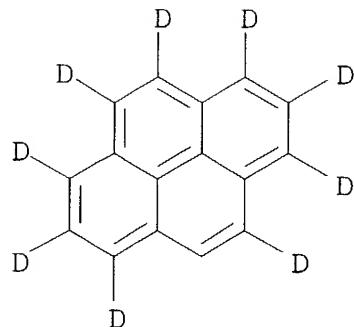
RN 167871-60-5 HCA

CN Pyrene-1,2,7-d3 (9CI) (CA INDEX NAME)

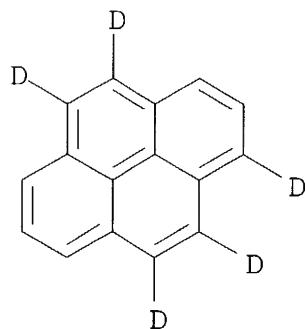


RN 167871-61-6 HCA

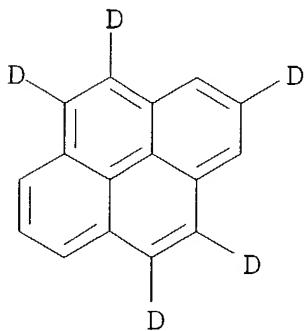
CN Pyrene-1,2,3,4,5,6,7,8,9-d9 (9CI) (CA INDEX NAME)



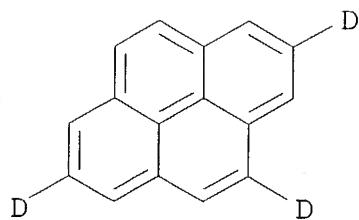
RN 169311-87-9 HCA
CN Pyrene-1,4,5,9,10-d5 (9CI) (CA INDEX NAME)



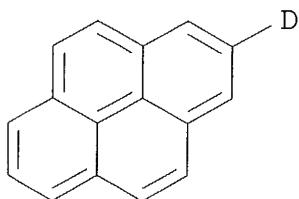
RN 169311-88-0 HCA
CN Pyrene-2,4,5,9,10-d5 (9CI) (CA INDEX NAME)



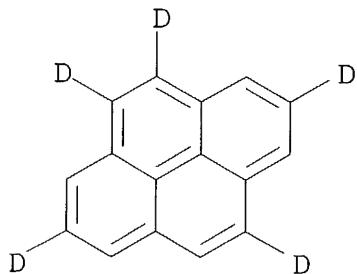
RN 174809-18-8 HCA
CN Pyrene-2,4,7-d3 (9CI) (CA INDEX NAME)



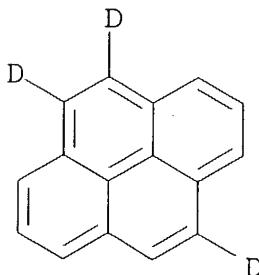
RN 174809-24-6 HCA
CN Pyrene-2-d (9CI) (CA INDEX NAME)



RN 174809-25-7 HCA
CN Pyrene-2,4,5,7,9-d5 (9CI) (CA INDEX NAME)

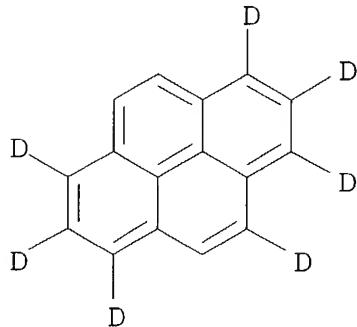


RN 174809-26-8 HCA
CN Pyrene-4,5,9-d3 (9CI) (CA INDEX NAME)



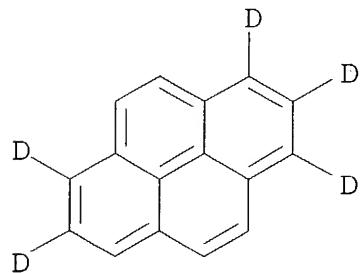
RN 174809-27-9 HCA

CN Pyrene-1,2,3,4,6,7,8-d7 (9CI) (CA INDEX NAME)



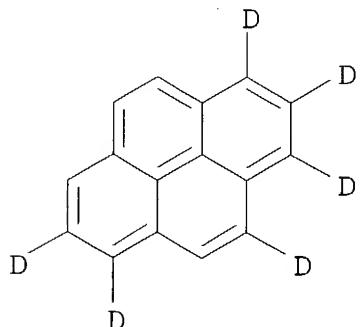
RN 174809-28-0 HCA

CN Pyrene-1,2,3,6,7-d5 (9CI) (CA INDEX NAME)



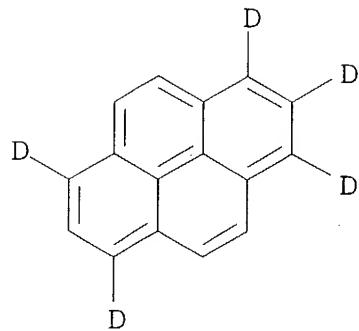
RN 174809-29-1 HCA

CN Pyrene-1,2,3,4,6,7-d6 (9CI) (CA INDEX NAME)

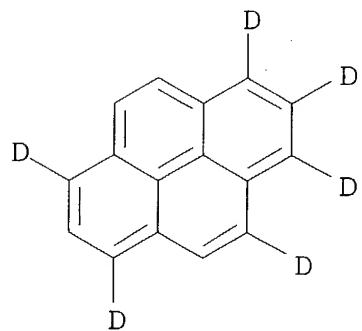


RN 174809-30-4 HCA

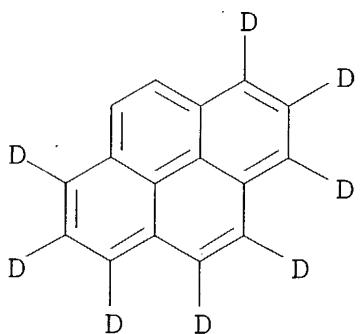
CN Pyrene-1,2,3,6,8-d5 (9CI) (CA INDEX NAME)



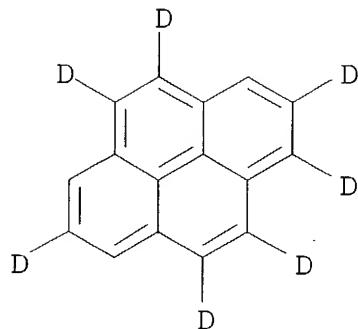
RN 174809-31-5 HCA
CN Pyrene-1,2,3,4,6,8-d6 (9CI) (CA INDEX NAME)



RN 174809-32-6 HCA
CN Pyrene-1,2,3,4,5,6,7,8-d8 (9CI) (CA INDEX NAME)

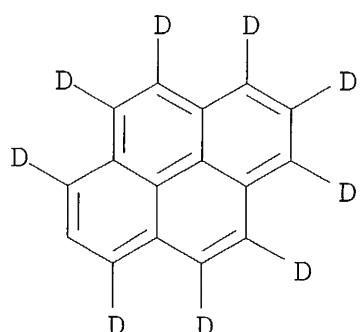


RN 174809-33-7 HCA
CN Pyrene-1,2,4,5,7,9,10-d7 (9CI) (CA INDEX NAME)



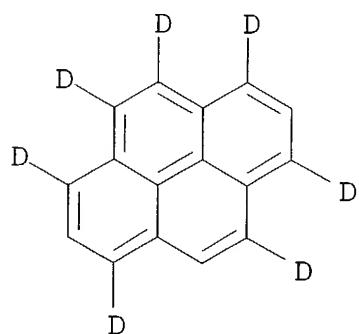
RN 174809-34-8 HCA

CN Pyrene-1,2,3,4,5,6,8,9,10-d9 (9CI) (CA INDEX NAME)



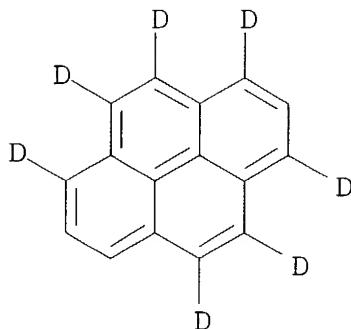
RN 174809-35-9 HCA

CN Pyrene-1,3,4,5,6,8,9-d7 (9CI) (CA INDEX NAME)

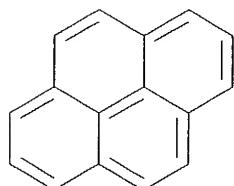


RN 174809-36-0 HCA

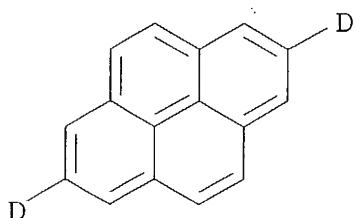
CN Pyrene-1,3,4,5,6,9,10-d7 (9CI) (CA INDEX NAME)



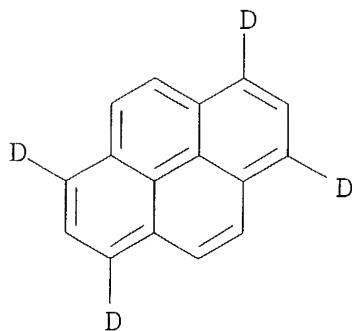
RN 174819-54-6 HCA
 CN Pyrene-d4 (9CI) (CA INDEX NAME)



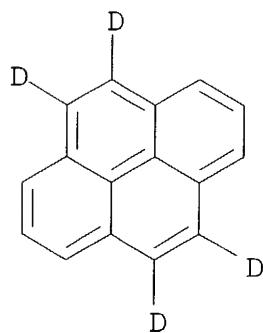
IT 174809-08-6 174809-09-7 174809-10-0
 174809-11-1 174809-12-2 174953-07-2
 (correlations between voltammetric, ESR, and semiempirical PM3
 calcns. and relative soln. electron affinities of selectively
 deuterated pyrenes)
 RN 174809-08-6 HCA
 CN Pyrene-2,7-d2, radical ion(1-) (9CI) (CA INDEX NAME)



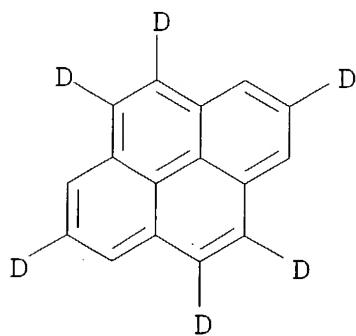
RN 174809-09-7 HCA
 CN Pyrene-1,3,6,8-d4, radical ion(1-) (9CI) (CA INDEX NAME)



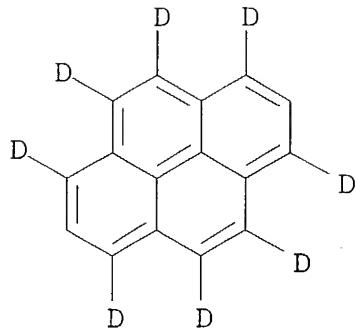
RN 174809-10-0 HCA
CN Pyrene-4,5,9,10-d4, radical ion(1-) (9CI) (CA INDEX NAME)



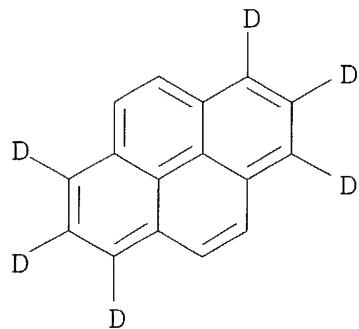
RN 174809-11-1 HCA
CN Pyrene-2,4,5,7,9,10-d6, radical ion(1-) (9CI) (CA INDEX NAME)



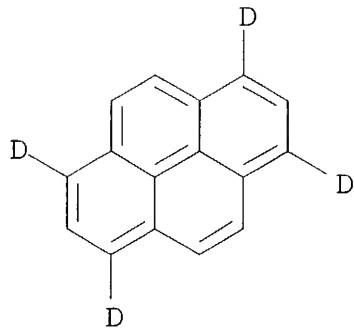
RN 174809-12-2 HCA
CN Pyrene-1,3,4,5,6,8,9,10-d8, radical ion(1-) (9CI) (CA INDEX NAME)



RN 174953-07-2 HCA
 CN Pyrene-1,2,3,6,7,8-d6, radical ion(1-) (9CI) (CA INDEX NAME)

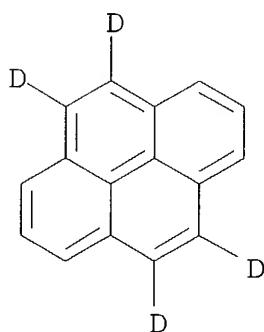


IT 78751-89-0P, Pyrene-1,3,6,8-d4 174809-13-3P,
 Pyrene-4,5,9,10-d4 174809-14-4P, Pyrene-1,2,3,6,7,8-d6
 174809-15-5P, Pyrene-2,4,5,7,9,10-d6 174809-16-6P,
 Pyrene-1,3,4,5,6,8,9,10-d8 174809-17-7P, Pyrene-2,7-d2
 (correlations between voltammetric, ESR, and semiempirical PM3
 calcns. and relative soln. electron affinities of selectively
 deuterated pyrenes)
 RN 78751-89-0 HCA
 CN Pyrene-1,3,6,8-d4 (9CI) (CA INDEX NAME)



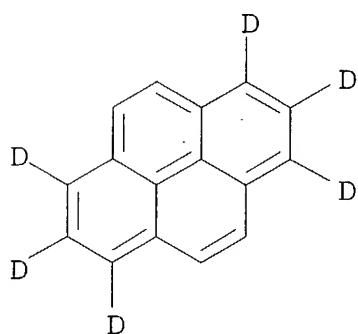
RN 174809-13-3 HCA

CN Pyrene-4,5,9,10-d4 (9CI) (CA INDEX NAME)



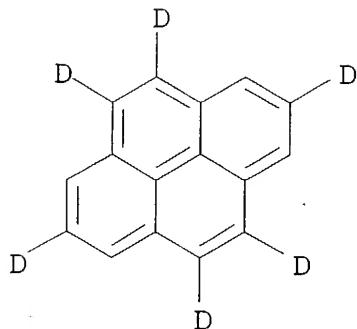
RN 174809-14-4 HCA

CN Pyrene-1,2,3,6,7,8-d6 (9CI) (CA INDEX NAME)



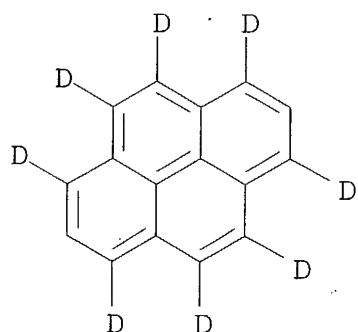
RN 174809-15-5 HCA

CN Pyrene-2,4,5,7,9,10-d6 (9CI) (CA INDEX NAME)



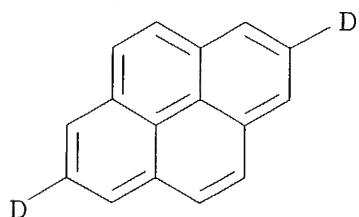
RN 174809-16-6 HCA

CN Pyrene-1,3,4,5,6,8,9,10-d8 (9CI) (CA INDEX NAME)



RN 174809-17-7 HCA

CN Pyrene-2,7-d2 (9CI) (CA INDEX NAME)

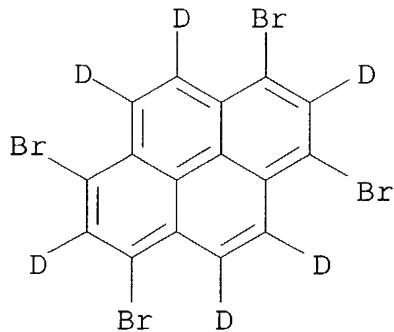


IT 174809-19-9P

(correlations between voltammetric, ESR, and semiempirical PM3 calcns. and relative soln. electron affinities of selectively deuterated pyrenes)

RN 174809-19-9 HCA

CN Pyrene-2,4,5,7,9,10-d6, 1,3,6,8-tetrabromo- (9CI) (CA INDEX NAME)



IT **167871-51-4P**, Pyrene-1,3,6-d3 **167871-60-5P**,
 Pyrene-1,2,7-d3 **167871-61-6P**, Pyrene-1,2,3,4,5,6,7,8,9-d9
169311-87-9P, Pyrene-1,4,5,9,10-d5 **169311-88-0P**,
 Pyrene-2,4,5,9,10-d5 **174809-18-8P**, Pyrene-2,4,7-d3
174809-24-6P, Pyrene-2-d **174809-25-7P**,
 Pyrene-2,4,5,7,9-d5 **174809-26-8P**, Pyrene-4,5,9-d3
174809-27-9P, Pyrene-1,2,3,4,6,7,8-d7 **174809-28-0P**
 , Pyrene-1,2,3,6,7-d5 **174809-29-1P**, Pyrene-1,2,3,4,6,7-d6
174809-30-4P, Pyrene-1,2,3,6,8-d5 **174809-31-5P**,
 Pyrene-1,2,3,4,6,8-d6 **174809-32-6P**, Pyrene-1,2,3,4,5,6,7,8-
 d8 **174809-33-7P**, Pyrene-1,2,4,5,7,9,10-d7
174809-34-8P, Pyrene-1,2,3,4,5,6,8,9,10-d9
174809-35-9P, Pyrene-1,3,4,5,6,8,9-d7 **174809-36-0P**
 , Pyrene-1,3,4,5,6,9,10-d7 **174819-54-6P**, Pyrene-d4
 (correlations between voltammetric, ESR, and semiempirical PM3
 calcns. and relative soln. electron affinities of selectively
 deuterated pyrenes)

IT **174809-08-6** **174809-09-7** **174809-10-0**
174809-11-1 **174809-12-2** **174953-07-2**
 (correlations between voltammetric, ESR, and semiempirical PM3
 calcns. and relative soln. electron affinities of selectively
 deuterated pyrenes)

IT **78751-89-0P**, Pyrene-1,3,6,8-d4 **174809-13-3P**,
 Pyrene-4,5,9,10-d4 **174809-14-4P**, Pyrene-1,2,3,6,7,8-d6
174809-15-5P, Pyrene-2,4,5,7,9,10-d6 **174809-16-6P**,
 Pyrene-1,3,4,5,6,8,9,10-d8 **174809-17-7P**, Pyrene-2,7-d2
 (correlations between voltammetric, ESR, and semiempirical PM3
 calcns. and relative soln. electron affinities of selectively
 deuterated pyrenes)

IT **174809-19-9P**
 (correlations between voltammetric, ESR, and semiempirical PM3
 calcns. and relative soln. electron affinities of selectively
 deuterated pyrenes)

123:198173 Perturbation of Spin Density Distribution Due to Deuterium Substitution. Zuilhof, Han; Lodder, Gerrit; van Mill, Robert P.; Mulder, Patrick P. J.; Kage, David E.; Reiter, Richard C.; Stevenson, Cheryl D. (Gorlaeus Laboratories, Leiden University, Leiden, 2300 RA, Neth.). Journal of Physical Chemistry, 99(11), 3461-4 (English) 1995. CODEN: JPCHAX. ISSN: 0022-3654. Publisher: American Chemical Society.

AB The EPR anal. of the anion radicals 1,3,6,8-tetradedeuteriopyrene and 1,3,4,5,6,8,9,10-octadedeuteriopyrene in THF with K⁺ at 173 K show that the obsd. coupling const. for the protons in the 2,7 positions is decreased in both anion radicals by 25 mG ($\Delta aH = -25$ mG) from its value in the anion radical of pyrene itself. This implies that there is only a very small, if any, contribution to this redn. in the spin d. at the 2,7 positions resulting from deuterium substitution in the 4,5,9,10 positions. Ab initio calcns. (6-31G** and 6-311G** basis sets) carried out considering the C-D bond to be shorter than the C-H bond by 0.01 Å predict the effects of octadedeuteriation to be 21 and 18 mG, resp., in good agreement with expt. The calcns. do, however, predict an approx. equal contribution from the two tetradedeuterio substitution patterns, with the effect of 1,3,6,8-deuteriation being slightly larger than that of 4,5,9,10-tetradedeuteriation.

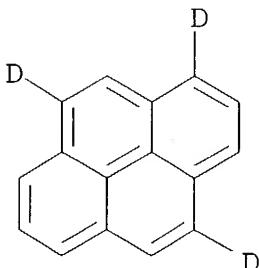
IT 167871-54-7P 167871-55-8P 167871-57-0P

167871-58-1P

(deuterium isotope effects on ESR and spin d. distributions of pyrene anion radicals)

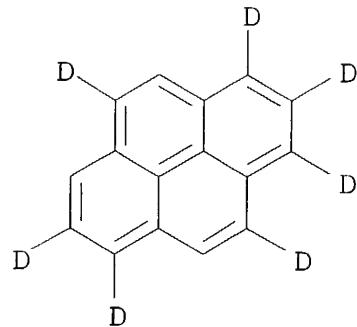
RN 167871-54-7 HCA

CN Pyrene-1,4,9-d3, radical ion(1-) (9CI) (CA INDEX NAME)



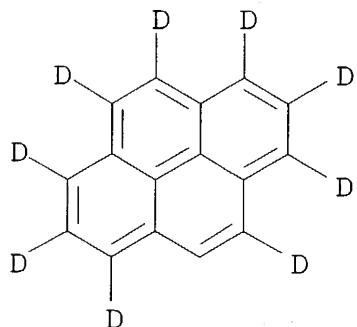
RN 167871-55-8 HCA

CN Pyrene-1,2,3,4,6,7,9-d7, radical ion(1-) (9CI) (CA INDEX NAME)



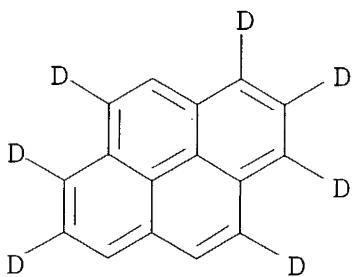
RN 167871-57-0 HCA

CN Pyrene-1,2,3,4,5,6,7,8,9-d9, radical ion(1-) (9CI) (CA INDEX NAME)



RN 167871-58-1 HCA

CN Pyrene-1,2,3,4,7,8,9-d7, radical ion(1-) (9CI) (CA INDEX NAME)



IT 167871-51-4P, Pyrene-1,3,6-d3 167871-60-5P,

Pyrene-1,2,7-d3 167871-61-6P, Pyrene-1,2,3,4,5,6,7,8,9-d9

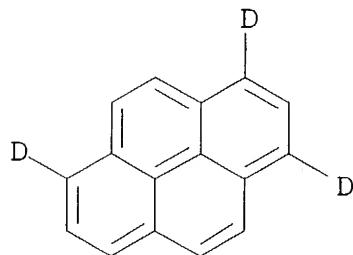
167871-62-7P, Pyrene-1,2,3,4,7,8,9-d7 167871-63-8P

, Pyrene-1,2,3,4,6,7,9-d7 169311-87-9P,

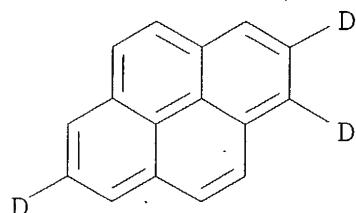
Pyrene-1,4,5,9,10-d5 169311-88-0P, Pyrene-2,4,5,9,10-d5

(deuterium isotope effects on ESR and spin d. distributions of pyrene anion radicals)

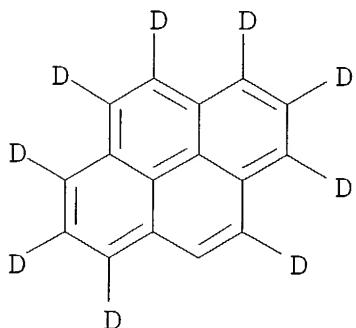
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CN Pyrene-1,3,6-d3 (9CI) (CA INDEX NAME)



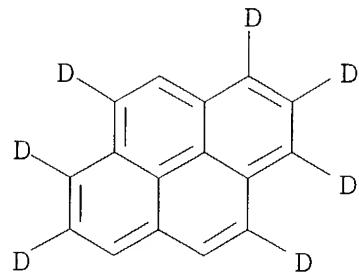
RN 167871-60-5 HCA
CN Pyrene-1,2,7-d3 (9CI) (CA INDEX NAME)



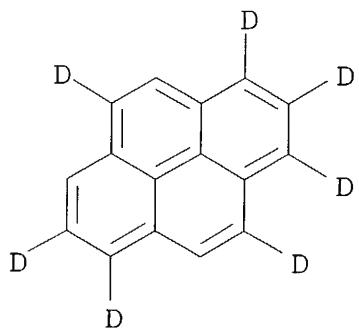
RN 167871-61-6 HCA
CN Pyrene-1,2,3,4,5,6,7,8,9-d9 (9CI) (CA INDEX NAME)



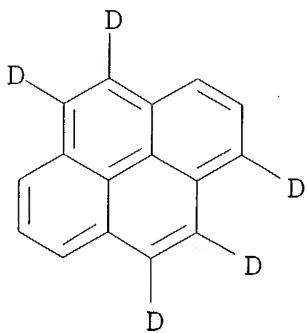
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CN Pyrene-1,2,3,4,7,8,9-d7 (9CI) (CA INDEX NAME)



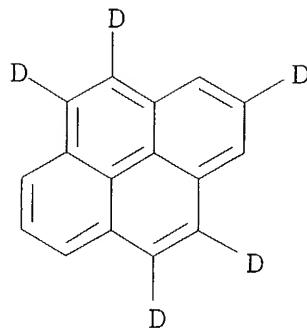
RN 167871-63-8 HCA
CN Pyrene-1,2,3,4,6,7,9-d7 (9CI) (CA INDEX NAME)



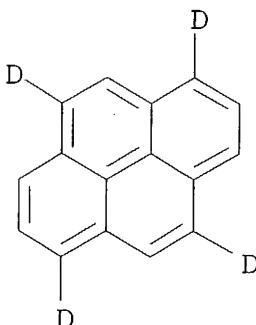
RN 169311-87-9 HCA
CN Pyrene-1,4,5,9,10-d5 (9CI) (CA INDEX NAME)



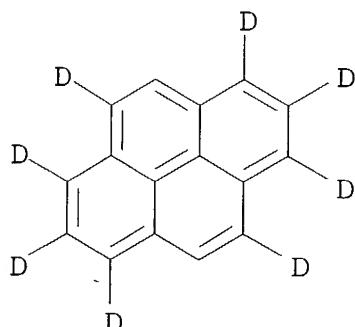
RN 169311-88-0 HCA
CN Pyrene-2,4,5,9,10-d5 (9CI) (CA INDEX NAME)



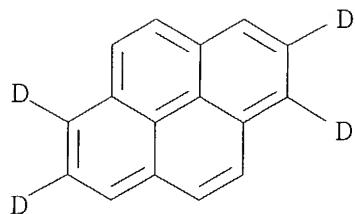
IT 167871-52-5P 167871-53-6P 167871-56-9P
 (deuterium isotope effects on ESR and spin d. distributions of
 pyrene anion radicals)
 RN 167871-52-5 HCA
 CN Pyrene-1,4,6,9-d4, radical ion(1-) (9CI) (CA INDEX NAME)



RN 167871-53-6 HCA
 CN Pyrene-1,2,3,4,6,7,8,9-d8, radical ion(1-) (9CI) (CA INDEX NAME)



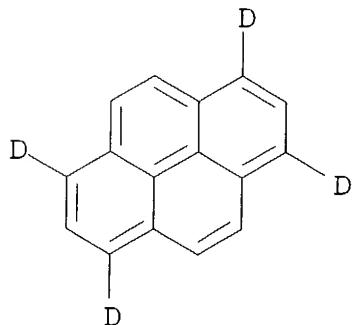
RN 167871-56-9 HCA
 CN Pyrene-1,2,6,7-d4, radical ion(1-) (9CI) (CA INDEX NAME)



IT 78751-89-0P, Pyrene-1,3,6,8-d4 167871-50-3P,
 Pyrene-1,2,4,5,6,7,9,10-d8 167871-64-9P, Pyrene-1,2,6,7-d4
 (deuterium isotope effects on ESR and spin d. distributions of
 pyrene anion radicals)

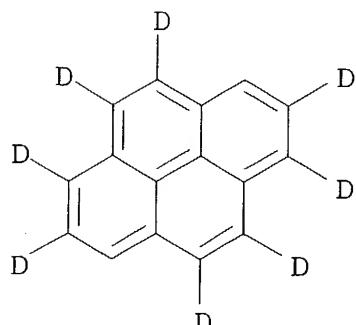
RN 78751-89-0 HCA

CN Pyrene-1,3,6,8-d4 (9CI) (CA INDEX NAME)



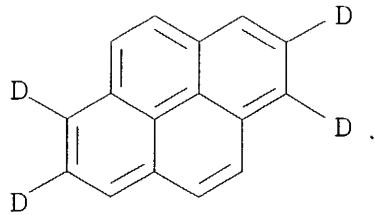
RN 167871-50-3 HCA

CN Pyrene-1,2,4,5,6,7,9,10-d8 (9CI) (CA INDEX NAME)



RN 167871-64-9 HCA

CN Pyrene-1,2,6,7-d4 (9CI) (CA INDEX NAME)



IT 167871-54-7P 167871-55-8P 167871-57-0P
167871-58-1P
 (deuterium isotope effects on ESR and spin d. distributions of pyrene anion radicals)

IT 167871-51-4P, Pyrene-1,3,6-d3 167871-60-5P,
 Pyrene-1,2,7-d3 167871-61-6P, Pyrene-1,2,3,4,5,6,7,8,9-d9
167871-62-7P, Pyrene-1,2,3,4,7,8,9-d7 167871-63-8P
 , Pyrene-1,2,3,4,6,7,9-d7 169311-87-9P,
 Pyrene-1,4,5,9,10-d5 169311-88-0P, Pyrene-2,4,5,9,10-d5
 (deuterium isotope effects on ESR and spin d. distributions of pyrene anion radicals)

IT 167871-52-5P 167871-53-6P 167871-56-9P
 (deuterium isotope effects on ESR and spin d. distributions of pyrene anion radicals)

IT 78751-89-0P, Pyrene-1,3,6,8-d4 167871-50-3P,
 Pyrene-1,2,4,5,6,7,9,10-d8 167871-64-9P, Pyrene-1,2,6,7-d4
 (deuterium isotope effects on ESR and spin d. distributions of pyrene anion radicals)

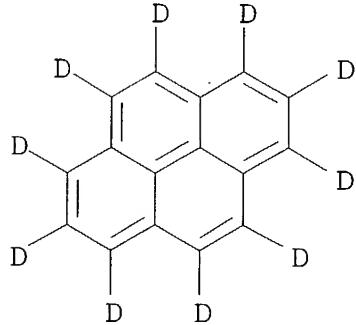
L25 ANSWER 12 OF 28 HCA COPYRIGHT 2004 ACS on STN
 122:172919 Infrared Spectroscopy of Matrix-Isolated Polycyclic Aromatic Hydrocarbon Cations. 2. The Members of the Thermodynamically Most Favorable Series through Coronene. Hudgins, D. M.; Allamandola, L. J. (Ames Research Center, NASA, Moffett Field, CA, 94035, USA). Journal of Physical Chemistry, 99(10), 3033-46 (English) 1995. CODEN: JPCHAX. ISSN: 0022-3654. Publisher: American Chemical Society.

AB Gaseous, ionized polycyclic arom. hydrocarbons (PAHs) probably are responsible for a very common family of interstellar IR emission bands. Here the near- and mid-IR spectra of the cations of the five most thermodynamically favored PAHs up to coronene, phenanthrene, pyrene, benzo[e]pyrene, benzo[ghi]perylene, and coronene, are presented to test this hypothesis. For those mols. that were studied previously (pyrene, pyrene-d10, and coronene), band positions and relative intensities are in agreement. In all of these cases the authors report addnl. features. Abs. integrated absorbance values are given for the phenanthrene, perdeuteriophenanthrene, pyrene, benzo[ghi]perylene, and coronene

cations. With the exception of coronene, the cation bands corresponding to the CC modes are typically 2-5 times more intense than those of the CH out-of-plane bending vibrations. For the cations, the CC stretching and CH in-plane bending modes give rise to bands that are an order of magnitude stronger than those of the neutral species, and the CH out-of-plane bends produce bands that are 5-20 times weaker than those of for the neutral species. This behavior is similar to that found in most other PAH cations studied to date. The astronomical implications of these PAH cation spectra are also discussed.

IT 159169-39-8
 (IR spectroscopy of matrix-isolated polycyclic arom. hydrocarbon cations)

RN 159169-39-8 HCA
 CN Pyrene-d10, radical ion(1+) (9CI) (CA INDEX NAME)



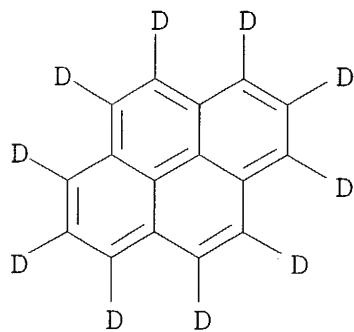
IT 159169-39-8
 (IR spectroscopy of matrix-isolated polycyclic arom. hydrocarbon cations)

L25 ANSWER 13 OF 28 HCA COPYRIGHT 2004 ACS on STN
 121:300360 Electronic and Vibrational Spectra Of Matrix-Isolated Pyrene Radical Cations: Theoretical and Experimental Aspects. Vala, Martin; Szczepanski, Jan; Pauzat, Francoise; Parisel, Olivier; Talbi, Dahbia; Ellinger, Yves (Department of Chemistry, University of Florida, Gainesville, FL, 32611-2046, USA). Journal of Physical Chemistry, 98(37), 9187-96 (English) 1994. CODEN: JPCHAX. ISSN: 0022-3654.

AB The radical cation of the polycyclic arom. hydrocarbon pyrene has been formed by vapor-phase electron impact, trapped in an argon matrix at 12 K, and its visible and IR spectra have been recorded. Integral intensities of both its electronic and vibrational bands have been detd. Comparison of the electronic absorption spectrum with previously reported argon- and neon-matrix-isolated spectra, vapor-phase photoelectron results, and multireference CI (MRCI) calcns. by using the PPP approach and a new INDO (INDO) formalism,

esp. developed for spectroscopic purposes, shows good agreement. Theor. frequencies and intensities of the vibrational modes have also been detd. using a RHF treatment with a 3-21G split-valence basis set. Significant differences between the IR intensities of neutral and cationic pyrene are predicted and substantiated exptl. IR absorption of perdeuterated pyrene radical cations has also been recorded and used to substantiate the proposed vibrational assignments.

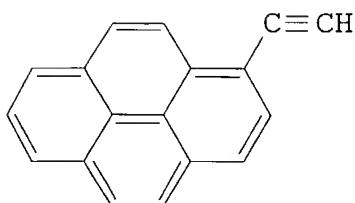
IT 159169-39-8, Pyrene-d10, radical ion(1+)
(matrix-isolated, IR and UV spectra and theor. calcns. of)
RN 159169-39-8 HCA
CN Pyrene-d10, radical ion(1+) (9CI) (CA INDEX NAME)



IT 159169-39-8, Pyrene-d10, radical ion(1+)
(matrix-isolated, IR and UV spectra and theor. calcns. of)

L25 ANSWER 14 OF 28 HCA COPYRIGHT 2004 ACS on STN
118:53725 Determinants of protein modification versus heme alkylation:
inactivation of cytochrome P450 1A1 by 1-ethynylpyrene and
phenylacetylene. Chan, William K.; Sui, Zhihua; Ortiz de
Montellano, Paul R. (Sch. Pharm., Univ. California, San Francisco,
CA, 94143-0446, USA). Chemical Research in Toxicology, 6(1), 38-45
(English) 1993. CODEN: CRTOEC. ISSN: 0893-228X.

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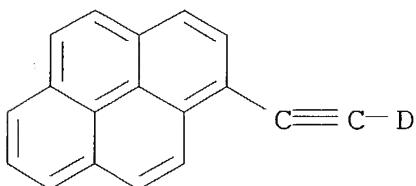
AB The authors have investigated the cytochrome P 4501A1-catalyzed oxidn. of 1-ethynylpyrene (1-EP) (I) and phenylacetylene (PA). Cytochrome P 4501A1 in microsomes from β -naphthoflavone-induced rats is inactivated in a time- and NADPH-dependent manner by 1-EP and PA. Parallel loss of the heme chromophore is obsd. with PA but not with 1-EP, although partial heme chromophore loss is obsd. when the purified, reconstituted enzyme is inactivated by either agent. Product anal. shows that 1-EP and PA are oxidized to, resp., (1'-pyrenyl)acetic and phenylacetic acids. In contrast to the inactivation of cytochrome P 4502B1 by PA, no isotope effect is obsd. on enzyme inactivation or metabolite formation when the acetylenic hydrogen is replaced by deuterium in either 1-EP or PA. Inactivation of cytochrome P 4501A1 by 1-EP results in covalent binding of 0.8-0.9 equiv (relative to total cytochrome P 450 content) of the inhibitor to the microsomal protein. The results demonstrate that a single isoenzyme can be inactivated, depending on the structure of the arylacetylene, by heme or protein alkylation. Spectroscopic binding consts. (Ks) show that 1-EP binds to the enzyme with >2000 times greater affinity than PA. This large difference in binding affinity is a probable factor in the heme vs. protein specificity of the inactivation reaction.

IT 144900-73-2P

(prepn. of)

RN 144900-73-2 HCA

CN Pyrene, 1-(ethynyl-d)- (9CI) (CA INDEX NAME)



IT 144900-73-2P
(prepn. of)

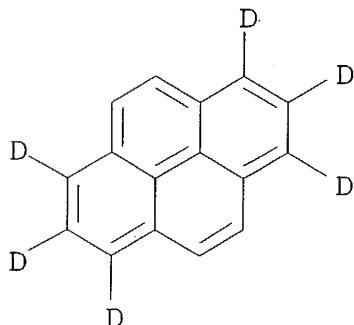
L25 ANSWER 15 OF 28 HCA COPYRIGHT 2004 ACS on STN

116:173438 ESR studies of deuterated polycyclic aromatic radical cations. Sang, Hong; Wang, Hanqing (Lanzhou Inst. Chem. Phys., Chin. Acad. Sci., Lanzhou, 730000, Peop. Rep. China). Magnetic Resonance in Chemistry, 30(2), 143-9 (English) 1992. CODEN: MRCHEG. ISSN: 0749-1581.

AB Several deuterated polycyclic arom. radical cations were studied by ESR. Their hyperfine coupling consts. are reported and mechanisms for their formation are proposed.

IT 124808-11-3P

RN (formation and ESR of)
 124808-11-3 HCA
 CN Pyrene-1,2,3,6,7,8-d6, radical ion(1+) (9CI) (CA INDEX NAME)



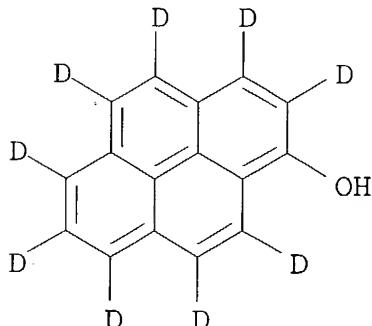
IT **124808-11-3P**
 (formation and ESR of)

L25 ANSWER 16 OF 28 HCA COPYRIGHT 2004 ACS on STN
 114:121608 A facile synthesis of 1-hydroxy-2-nitropyrene and its applicability to other ortho-substituted hydroxynitroarenes. Zielinska, Barbara (Energy Environ. Eng. Cent., Desert Res. Inst., Reno, NV, 89506, USA). Polycyclic Aromatic Compounds, 1(4), 207-11 (English) 1990. CODEN: PARCEO. ISSN: 1040-6638. OTHER SOURCES: CASREACT 114:121608.

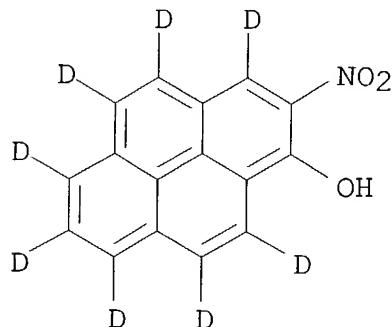
AB The use of 4-nitro-4-ethyl-2,3,5,6-tetrabromo-1,4-cyclohexadien-1-one (I) as nitrating agent for hydroxyarenes was discussed. Thus, the regioselective nitration of 1-hydroxypyrene with I gave 80% 1-hydroxy-2-nitropyrene.

IT **132603-37-3P**, 1-Hydroxypyrene-d9
 (prepn. and nitration of, with nitroethyltetrabromocyclohexadiene, regioselective)

RN 132603-37-3 HCA
 CN 1-Pyren-2,3,4,5,6,7,8,9,10-d9-ol (9CI) (CA INDEX NAME)



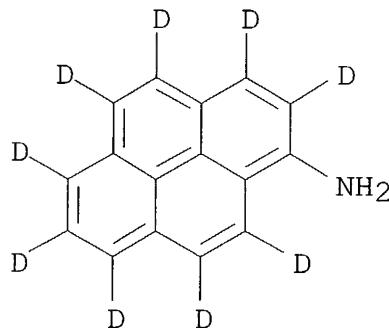
IT 132603-38-4P, 1-Hydroxy-2-nitropyrene-d8
(prepn. of)
RN 132603-38-4 HCA
CN 1-Pyren-3,4,5,6,7,8,9,10-d8-ol, 2-nitro- (9CI) (CA INDEX NAME)



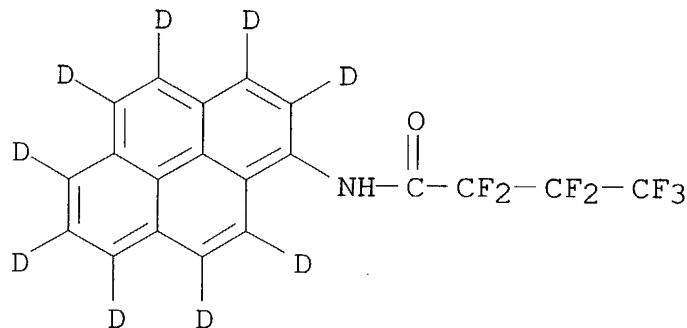
IT 132603-37-3P, 1-Hydroxypyrene-d9
(prepn. and nitration of, with nitroethyltetrabromocyclohexadieno-
ne, regioselective)
IT 132603-38-4P, 1-Hydroxy-2-nitropyrene-d8
(prepn. of)

L25 ANSWER 17 OF 28 HCA COPYRIGHT 2004 ACS on STN
113:35955 Selection of electrophoric derivatives of 1-aminopyrene and
2-aminofluorene for determination by gas chromatography with
electron-capture negative-ion mass spectrometry. Bakthavachalam,
Jothi; Annan, Roland S.; Beland, Frederick A.; Vouros, Paul; Giese,
Roger W. (Barnett Inst. Chem., Northeastern Univ., Boston, MA,
02115, USA). Journal of Chromatography, 500, 373-86 (English) 1990.
CODEN: JOCRAM. ISSN: 0021-9673. OTHER SOURCES: CASREACT 113:35955.
AB Several electrophoric derivs. of 1-aminopyrene and 2-aminofluorene
were prep'd. Reagents such as heptafluorobutyryl chloride,
pentafluorobenzoyl chloride, pentafluorobenzyl bromide and
pentafluorobenzaldehyde, alone and in certain combinations, were
employed. The ease of formation, yield, stability and fragmentation
by gas chromatog. with electron-capture neg.-ion (ECNI) mass
spectrometry of the derivs. were compared. This allowed the most
promising ones to be selected for future work on the sensitive
detection of aminopolyaroms. by this detection technique.
Pentafluorobenzylidene (first choice) and N-pentafluorobenzyl-N-
heptafluorobutyryl (second choice) derivs. emerged as the best ones.
The origins of loss of HF and 2HF from some of the derivs. were
elucidated in the ECNI mass spectra by studies of deuterium-labeled
analogs.
IT 128008-86-6P, 1-Pyren-2,3,4,5,6,7,8,9,10-d9-amine
(prepn. and derivatization of, for gas chromatog. with
electron-capture neg.-ion mass spectrometry)

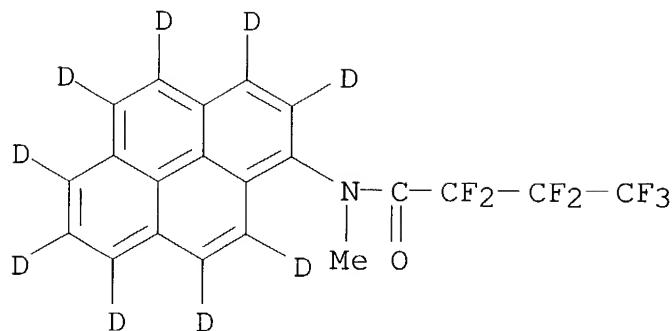
RN 128008-86-6 HCA
 CN 1-Pyren-2,3,4,5,6,7,8,9,10-d9-amine (9CI) (CA INDEX NAME)



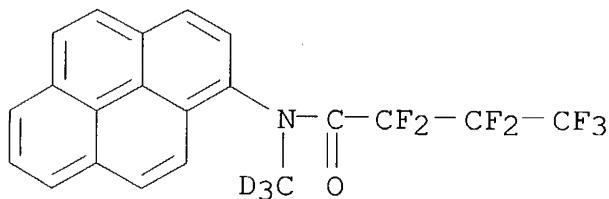
IT 128008-89-9P 128008-91-3P 128008-93-5P
 (prepn. and gas chromatog.-electron-capture neg.-ion mass
 spectrometry of)
 RN 128008-89-9 HCA
 CN Butanamide, 2,2,3,3,4,4,4-heptafluoro-N-(1-pyrenyl-
 2,3,4,5,6,7,8,9,10-d9)- (9CI) (CA INDEX NAME)



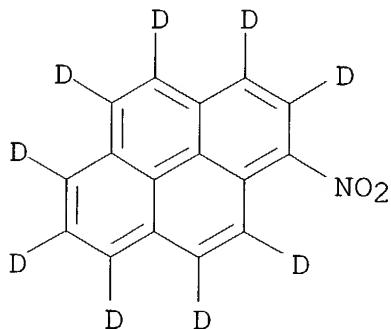
RN 128008-91-3 HCA
 CN Butanamide, 2,2,3,3,4,4,4-heptafluoro-N-methyl-N-(1-pyrenyl-
 2,3,4,5,6,7,8,9,10-d9)- (9CI) (CA INDEX NAME)



RN 128008-93-5 HCA
 CN Butanamide, 2,2,3,3,4,4,4-heptafluoro-N-(methyl-d3)-N-1-pyrenyl-
 (9CI) (CA INDEX NAME)



IT 93487-20-8P
 (prepn. and redn. of)
 RN 93487-20-8 HCA
 CN Pyrene-1,2,3,4,5,6,7,9,10-d9, 8-nitro- (9CI) (CA INDEX NAME)



IT 128008-86-6P, 1-Pyren-2,3,4,5,6,7,8,9,10-d9-amine
 (prepn. and derivatization of, for gas chromatog. with
 electron-capture neg.-ion mass spectrometry)
 IT 128008-89-9P 128008-91-3P 128008-93-5P
 (prepn. and gas chromatog.-electron-capture neg.-ion mass
 spectrometry of)

IT 93487-20-8P
(prepn. and redn. of)

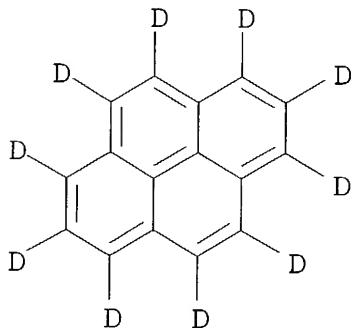
L25 ANSWER 18 OF 28 HCA COPYRIGHT 2004 ACS on STN
113:22957 Effect of charge distribution upon condensed-phase electron transfer between isotopic isomers. Stevenson, Gerald R.; Sturgeon, Bradley E. (Dep. Chem., Illinois State Univ., Normal, IL, 61761, USA). Journal of Organic Chemistry, 55(13), 4090-3 (English) 1990. CODEN: JOCEAH. ISSN: 0022-3263.

AB EPR anal. of anion radicals resulting from the partial K redn. mixts. of perdeuterated and perprotiated polyaroms. in THF show that the equil. const. for the reaction $R\bullet\bullet, M+ + *R = R + *R\bullet\bullet, M+$ is less than unity but that it is closer to unity for systems with large amts. of charge d. on the ring juncture carbons. These EPR results predict that sepn. of anion radical from neutral mol. would effect an isotopic sepn. Removal of THF leaves a solid mixt. of neutral polyarom. and the potassium anion-radical salt. Subsequent dissoln. or sublimation of the neutral polyaroms. from the anion radical yields a mixt. that is enriched in the heavy isotopic isomer, and reoxidn. of the anion radical with iodine yields a mixt. that is depleted in the heavy isotopic isomer. The room-temp. equil. consts. obtained from these phys. sepns. are not as large as those measured in soln. due to lattice effects in the solid state.

IT 127619-33-4P
(generation and ESR spectrum of)

RN 127619-33-4 HCA

CN Pyrene-d10, radical ion(1-) (9CI) (CA INDEX NAME)



IT 127619-33-4P
(generation and ESR spectrum of)

L25 ANSWER 19 OF 28 HCA COPYRIGHT 2004 ACS on STN
112:54822 An ESR investigation of radical cations formed in Friedel-Crafts reactions. Wang, Hanqing; Kispert, Lowell D.; Sang, Hong (Dep. Chem., Univ. Alabama, Tuscaloosa, AL, 35487, USA). Journal of the Chemical Society, Perkin Transactions 2: Physical

Organic Chemistry (1972-1999) (10), 1463-9 (English) 1989. CODEN: JCPKBH. ISSN: 0300-9580.

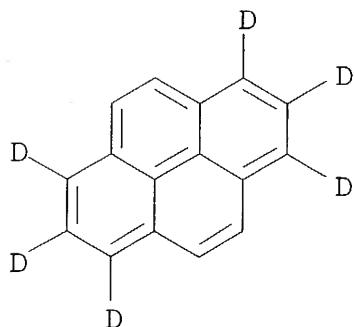
AB The detection and identification of radical cations produced in a Friedel-Crafts alkylating system, with benzene, toluene, or ethylbenzene, and an alkyl chloride is described. The obsd. ESR spectra are due to polycyclic arom. radical cations formed from the parent hydrocarbons. Benzyl halides produced in the Friedel-Crafts alkylating reaction undergo Scholl self-condensation to give polycyclic arom. hydrocarbons, which are converted into the corresponding polycyclic arom. radical cations in the presence of aluminum chloride.

IT **124808-11-3P**

(formation and ESR of)

RN 124808-11-3 HCA

CN Pyrene-1,2,3,6,7,8-d6, radical ion(1+) (9CI) (CA INDEX NAME)



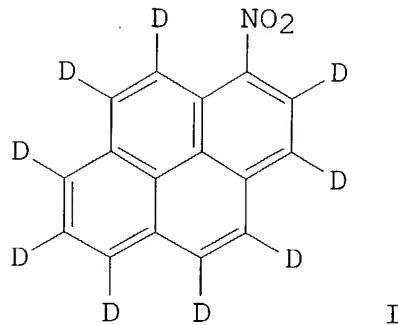
IT **124808-11-3P**

(formation and ESR of)

L25 ANSWER 20 OF 28 HCA COPYRIGHT 2004 ACS on STN

111:57233 Facile synthesis of 1-nitropyrene-d9 of high isotopic purity. Fatiadi, Alexander J.; Hilpert, Laurence R. (Org. Anal. Res. Div., Cent. Anal. Chem., Gathersburg, MD, 20899, USA). Journal of Labelled Compounds and Radiopharmaceuticals, 27(2), 129-36 (English) 1989. CODEN: JLCRD4. ISSN: 0362-4803. OTHER SOURCES: CASREACT 111:57233.

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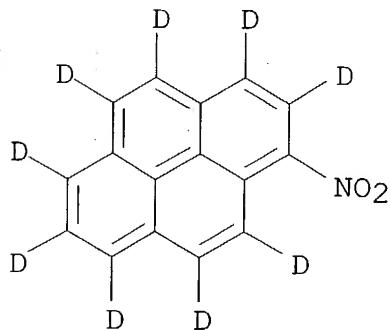


AB 1-Nitropyrene-d9 (I), 1,3-dinitropyrene-d8, 1,6-dinitropyrene-d8, and 1,8-dinitropyrene-d8, used as internal stds. for the detn. of nitropolycyclic arom. hydrocarbons (NPAH) in simple and complex mixts., and required for GC/MS measurements used in the certification of NBS Std. Ref. Material (SRM) 1596 (a mixt. of nitropyrenes), were synthesized in one step from com. available pyrene-d10 and nitric acid-d1. The electron impact mass spectra and isotopic purity of 1-nitropyrene-d9 and the deuterated dinitropyrenes were detd.; the compds. were characterized by gas chromatog.-mass spectrometry (GC-MS) and by high performance liq. chromatog. (HPLC). Caution: 1-nitropyrene-d9 is a potent mutagen.

IT 93487-20-8P 121700-13-8P 121700-14-9P
 121700-15-0P
 (prep. of)

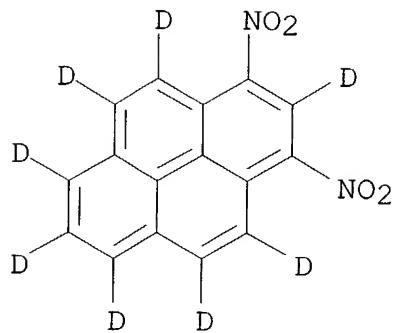
RN 93487-20-8 HCA

CN Pyrene-1,2,3,4,5,6,7,9,10-d9, 8-nitro- (9CI) (CA INDEX NAME)



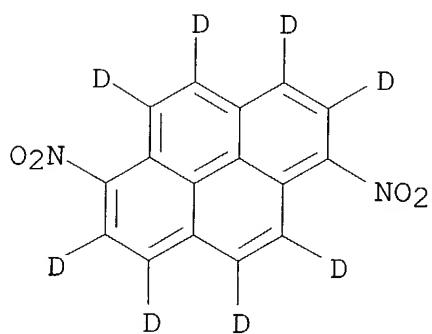
RN 121700-13-8 HCA

CN Pyrene-1,2,3,4,5,7,9,10-d8, 6,8-dinitro- (9CI) (CA INDEX NAME)



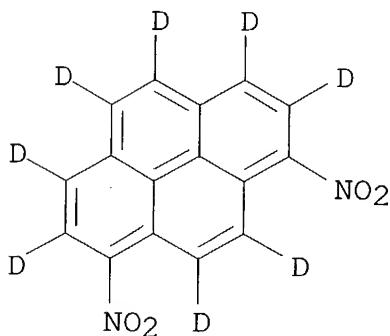
RN 121700-14-9 HCA

CN Pyrene-1,2,4,5,6,7,9,10-d8, 3,8-dinitro- (9CI) (CA INDEX NAME)



RN 121700-15-0 HCA

CN Pyrene-1,2,4,5,7,8,9,10-d8, 3,6-dinitro- (9CI) (CA INDEX NAME)



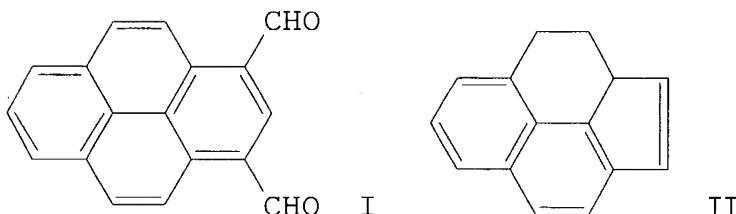
IT 93487-20-8P 121700-13-8P 121700-14-9P

121700-15-0P

(prep. of)

111:7037 A convenient synthesis of 1,3-pyrenedicarbaldehyde. Goltz, Michael; Murata, Ichiro (Fac. Sci., Osaka Univ., Toyonaka, 560, Japan). Bulletin of the Chemical Society of Japan, 61(10), 3767-9 (English) 1988. CODEN: BCSJA8. ISSN: 0009-2673. OTHER SOURCES: CASREACT 111:7037.

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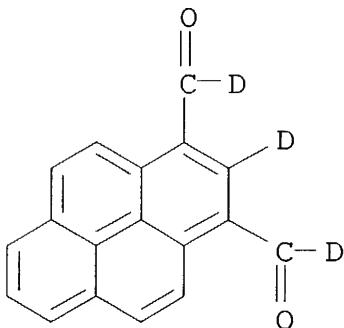


AB A convenient and preparatively useful access to the unknown 1,3-pyrenedicarboxaldehyde (I) is presented. When treated with an excess amt. of DMF and POCl_3 , 3,4-dihydro-2aH-cyclopenta[cd]phenalene (II) was smoothly converted into dialdehyde I in 57% yield. A plausible mechanism for this transformation was suggested from a labeling expt. using DMF-d7.

IT 120915-15-3P, 1,3-Pyrene-2-di (carboxaldehyde-d)
(prepn. of)

RN 120915-15-3 HCA

CN 1, 3-Pyrene-2-d-di(carboxaldehyde-d) (9CI) (CA INDEX NAME)



IT 120915-15-3P, 1,3-Pyrene-2-di (carboxaldehyde-d)
(prepn. of)

L25 ANSWER 22 OF 28 HCA COPYRIGHT 2004 ACS on STN
101:239628 Analysis of 1- and 4-nitropyrene and 1-nitropyrene-d9 via

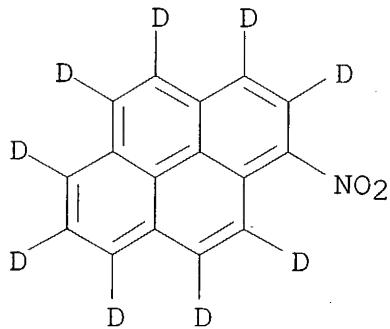
fused silica GC combined with negative ion atmospheric pressure ionization mass spectrometry. Korfomacher, W. A.; Miller, D. W. (Dep. Health Hum. Serv., Natl. Cent. Toxicol. Res., Jefferson, AR, 72079, USA). HRC & CC, Journal of High Resolution Chromatography and Chromatography Communications, 7(10), 581-3 (English) 1984. CODEN: HCJCDB. ISSN: 0344-7138.

AB The suitability of fused silica capillary gas chromatog. (GC) combined with ionization mass spectrometry was studied for detg. nitropyrenes. An SE 54-coated fused SiO₂ column and He carrier gas were used. A detection limit of 0.5 pg was achieved for 1-nitropyrene.

IT 93487-20-8
(detn. of, by capillary gas chromatog. combined with ionization mass spectrometry)

RN 93487-20-8 HCA

CN Pyrene-1,2,3,4,5,6,7,9,10-d₉, 8-nitro- (9CI) (CA INDEX NAME)



IT 93487-20-8
(detn. of, by capillary gas chromatog. combined with ionization mass spectrometry)

L25 ANSWER 23 OF 28 HCA COPYRIGHT 2004 ACS on STN
96:67940 Structure-resonance theory and the kinetics of the electrophilic deuterium-hydrogen exchange in benzenoid hydrocarbons. Shawali, Ahmad S.; Parkanyi, Cyril; Herndon, William C. (Fac. Sci., Univ. Cairo, Giza, Egypt). Journal of Organic Chemistry, 47(4), 734-6 (English) 1982. CODEN: JOCEAH. ISSN: 0022-3263.

AB Logarithms of the rates of deuterioprotonation of nine alternant hydrocarbons and of the protodedeuteration of various sites of five other benzenoid hydrocarbons have LFER with the cor. structure counts of the intermediate (\ln SCI), and the reactant (\ln SCR), and with their ratio [\ln (SCI/SCR)]. The differences in reactivity of benzenoid hydrocarbons in arom. substitution reactions are due to differences in their resonance energies; stabilization of the reaction intermediates by hyperconjugation is insignificant. The LFER of rate data vs. structure-resonance theory calcns. are better

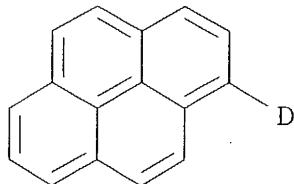
than those localization energies.

IT **6747-66-6**

(hydrogen exchange reaction of, structure-resonance theory in relation to kinetics of)

RN 6747-66-6 HCA

CN Pyrene-1-d (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **6747-66-6**

(hydrogen exchange reaction of, structure-resonance theory in relation to kinetics of)

L25 ANSWER 24 OF 28 HCA COPYRIGHT 2004 ACS on STN

95:96395 Infrared spectra of pyrene derivatives. Relation to the substitution pattern. Hansen, Poul Erik; Berg Arne (Dep. Org. Chem., Univ. Aarhus, Arhus, DK-8000, Den.). Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry, B 35(2), 131-7 (English) 1981. CODEN: ACBOCV. ISSN: 0302-4369.

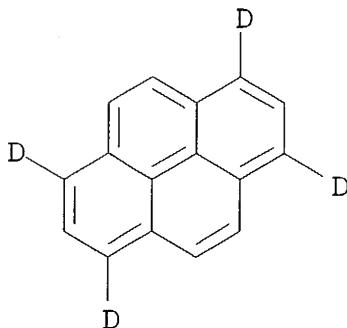
AB The IR of one-hundred and thirty-seven pyrene derivs. with 21 different types of substitution patterns are examd. and a set of empirical rules based on band positions and intensities are formulated which allow most types of pyrene derivs. to be structurally assigned. The examn. of 1-, 1,3-, 1,6-, 1,8- and 1,3,6,8-substituted pyrenes are used to reassign the 680 cm⁻¹ band to an Au species.

IT **78751-89-0**

(IR spectrum of)

RN 78751-89-0 HCA

CN Pyrene-1,3,6,8-d4 (9CI) (CA INDEX NAME)



IT **78751-89-0**
(IR spectrum of)

L25 ANSWER 25 OF 28 HCA COPYRIGHT 2004 ACS on STN
82:163520 Liquid nitrogen temperature study of the pyrene-d8-Tetracyanoethylene charge-transfer complex. Larsen, F. Krebs; Little, R. G.; Coppens, P. (Dep. Chem., State Univ. New York, Buffalo, NY, USA). Acta Crystallographica, Section B: Structural Crystallography and Crystal Chemistry, B31(2), 430-40 (English) 1975. CODEN: ACBCAR. ISSN: 0567-7408.

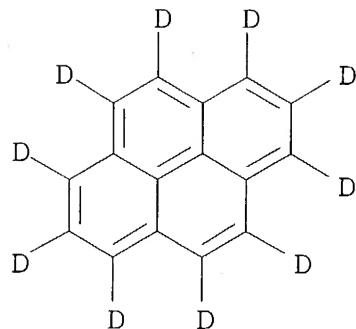
AB A liq.-N temp. diffraction anal. of the charge-transfer complex pyrene-d8-tetracyanoethylene is described. The cell parameters at 105°K are a 14.136(5), b 7.169(2), c 7.866(2) Å, and β 91.73(2)°. Although the data refine easily to $R(F) = 5.1\%$ and $Rw(F) = 3.8\%$, difference maps indicate disorder in the plane of the tetracyanoethylene (TCNE) mol. Subsequent refinement with 2 superimposed TCNE mols., whose geometries were constrained to be equal and whose thermal motion was restricted to rigid-body motion, converged at $R(F) = 4.7\%$ and $Rw(F) = 3.6\%$, showing an arrangement of TCNE mols. in 2 orientations with a relative rotation of 90° around the center of the mol. in the mol. plane. 7% of the mols. are in the alternative orientation which corresponds to an energy difference of at least 0.54 kcal mole-1. Comparison of the geometries of the component mols. with those in the noncomplexed crystals indicates effects of complexing on bond lengths to be at, or smaller than, the limit of exptl. accuracy. Integration of the charge d. over the vol. of the TCNE mol. shows the transfer of charge between the mols. in the crystal to be very small (<0.15e). This conclusion is confirmed by a refinement of the occupancy of the spherical valence shells of the constituent atoms.

IT **55157-63-6**
(crystal structure of)

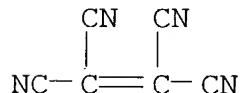
RN 55157-63-6 HCA
CN Ethenetetracarbonitrile, compd. with pyrene-d10 (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 1718-52-1
CMF C16 D10



CM 2

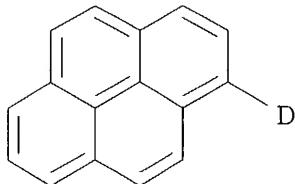
CRN 670-54-2
CMF C6 N4IT 55157-63-6
(crystal structure of)

L25 ANSWER 26 OF 28 HCA COPYRIGHT 2004 ACS on STN
 59:61358 Original Reference No. 59:11211c-d Rates of exchange of aryl hydrogens with lithium cyclohexylamide in cyclohexylamine.
 Streitwieser, A., Jr.; Lawler, R. G. (Univ. of California, Berkeley). Journal of the American Chemical Society, 85(18), 2854-5 (Unavailable) 1963. CODEN: JACSAT. ISSN: 0002-7863.

AB The rates of H isotope exchange of a no. of specifically deuterated and tritiated arenes with Li cyclohexylamide in C₆H₁₁NH₂ were detd. (CA 56, 15385g). Exchange occurred via the aryllithium intermediate, and the following conclusions were proposed, based on the assumption that the exchange rates were valid measures of the relative stabilities of the corresponding aryl anions: the greater exchange rate of the 3-biphenyl position over the 4-position indicated that carbene-carbanion resonance was not important in these cases; the perturbation of the π -electron system due to a change in Coulomb integral by the presence of a neg. charge on C appeared to be of minor importance.

IT 6747-66-6, Pyrene-1-d
(reaction with (cyclohexylamino)lithium)

RN 6747-66-6 HCA
CN Pyrene-1-d (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 6747-66-6, Pyrene-1-d
(reaction with (cyclohexylamino)lithium)

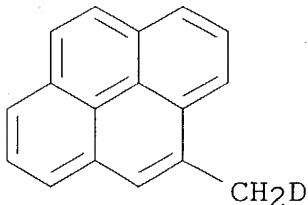
L25 ANSWER 27 OF 28 HCA COPYRIGHT 2004 ACS on STN
59:15012 Original Reference No. 59:2619c Acidity of hydrocarbons. VII.
Rates of exchange of polycyclic methylarene- α -d's with lithium
cyclohexylamide. Streitwieser, A., Jr.; Langworthy, W. C. (Univ. of
California, Berkeley). Journal of the American Chemical Society,
85, 1757-61 (Unavailable) 1963. CODEN: JACSAT. ISSN: 0002-7863.

AB cf. CA 58, 5469c. Rates of exchange are reported for various
deuteriomethyl derivs. of naphthalene, phenanthrene, anthracene,
pyrene, and fluoranthene with lithium cyclohexylamide in
cyclohexylamine at 49.9°. The relative rates are discussed
with reference to the stabilities of corresponding arylmethyl anions
and are compared with those of related carbonium ion reactions.

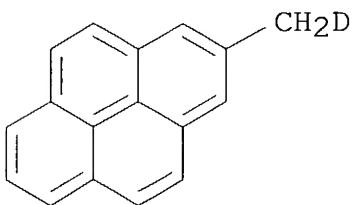
IT 98030-02-5, Pyrene, 4-methyl-d- 98030-03-6,
Pyrene, 2-methyl-d-
(reaction with (cyclohexylamino)lithium)

RN 98030-02-5 HCA

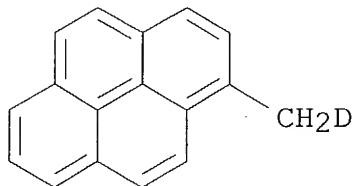
CN Pyrene, 4-methyl-d- (7CI) (CA INDEX NAME)



RN 98030-03-6 HCA
CN Pyrene, 2-methyl-d- (7CI) (CA INDEX NAME)



IT 98030-04-7, Pyrene, 1-methyl-d-
 (reaction with (cyclohexylamino)lithium, kinetics of)
 RN 98030-04-7 HCA
 CN Pyrene, 1-methyl-d- (7CI) (CA INDEX NAME)



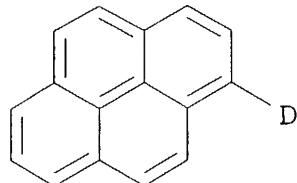
IT 98030-02-5, Pyrene, 4-methyl-d- 98030-03-6,
 Pyrene, 2-methyl-d-
 (reaction with (cyclohexylamino)lithium)
 IT 98030-04-7, Pyrene, 1-methyl-d-
 (reaction with (cyclohexylamino)lithium, kinetics of)

L25 ANSWER 28 OF 28 HCA COPYRIGHT 2004 ACS on STN
 53:38043 Original Reference No. 53:6770a-d Electron spin resonance
 spectra of aromatic mononegative and monopositive ions. de Boer,
 E.; Weissman, S. I. (Washington Univ., St. Louis, MO). Journal of
 the American Chemical Society, 80, 4549-55 (Unavailable) 1958.
 CODEN: JACSAT. ISSN: 0002-7863.
 AB Spectra of the mononegative ions of anthracene (I), tetracene (II),
 phenanthrene, biphenyl, terphenyl, perylene (III), pyrene (IV),
 triphenylene, coronene, fluoranthene (V), acenaphthylene (VI),
 acepleiadylene (VII), acenaphthene (VIII), and acepleiadiene (IX)
 are reported; also, spectra of the pos. ions of I, II, III, VII, and
 IX. The spectra are compared with those calcd. on the assumption of
 a linear relation between hyperfine coupling const. with a proton
 and the π -spin d. on the adjacent C. The latter were calcd. by a
 single configuration Huckel mol. orbital treatment. The spectra of
 the neg. ions of all the alternant hydrocarbons except IV are in
 agreement with the calcns.; so are those of the nonalternant V and
 VI, but not of VII. Among the pos. ions, agreement is found for I,
 II, and III, but not for IX. The ions of the partially satd. VIII
 and IX have high coupling consts. with the CH₂ protons and are not
 satisfactorily treated by simple mol. orbital theory. The anions
 were prep'd. with K in tetrahydrofuran, the cations in concd. H₂SO₄.
 Biphenyl-p-d, pyrene-3-d, and pyrene-3,5,8,10-d₄, prep'd. from the
 respective bromo compds., gave unchanged optical spectra but the
 expected differences of about 4 oersteds per D in the spin resonance
 spectra.
 IT 6747-66-6, Pyrene-1-d 132569-01-8,
 Pyrene-1,4,6,9-d₄

(magnetic resonance absorption by)

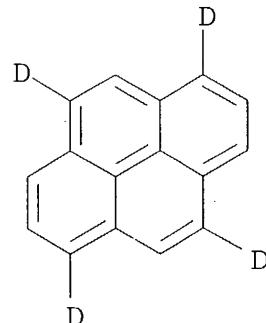
RN 6747-66-6 HCA

CN Pyrene-1-d (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 132569-01-8 HCA

CN Pyrene-1,4,6,9-d4 (6CI) (CA INDEX NAME)



IT 6747-66-6, Pyrene-1-d 132569-01-8,

Pyrene-1,4,6,9-d4

(magnetic resonance absorption by)